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Summaries of BFRL Fire Research In-House Projects and Grants, 1991

Nora H. Jason, Editor

United States Department of Commerce
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October 1991

U.S. Department of Commerce
Robert A. Mosbacher, *Secretary*
National Institute of Standards and Technology
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Gaithersburg, MD 20899

PREFACE

This report describes the fire research projects performed in the Building and Fire Research Laboratory (BFRL) and under its grants program during Fiscal Year 1991.

The BFRL is nationally recognized as the focal point for fire research in the United States of America and has a state-of-the-art multidisciplinary technical staff that is supported by an excellent fire library and extensive laboratory facilities.

The Federal Fire Prevention and Control Act of 1974 authorized the Secretary of Commerce to conduct a fire research program directly or through contracts and grants. Therefore, in addition to its in-house programs, the BFRL maintains a fire research grants program that supplements its in-house programs and through which supports most of the academic fire research in the United States. BFRL, as a component of the National Institute of Standards and Technology (NIST), responds to the needs of other Federal agencies and private sector organizations. This report covers work performed both with funds appropriated to the BFRL fire research program and under contract to other agencies.

The goal of the fire research program is to provide the technical basis for the reduction of losses and costs of fire. The program is designed to meet the fire safety needs of the public, the fire services, and the manufacturing industry by upgrading the knowledge of fire and of the measurement and prediction of the performance of products in fires. It is comprised of three elements:

* Basic research leading to the development of tools for "engineered fire safety", i.e., fire protection technologies and fire prediction methods;

* timely response to current fire problems, e.g., hazards of upholstered furniture, burning oil spills;

* focal point for fire research in the United States by incorporating in its program academic and international Visiting Scientists, working with academia on the development of fire-related training programs, participating in standards and codes organizations, operating a fire research information service and a computer bulletin board.

The majority of the in-house priority projects and grants work fits into the first category, basic research and tools for engineered fire safety, and is presented in Part 1 of this report. Work for other agencies fits in the second category, timely response to current fire problems, and is presented in Part 2. Activities under the third element are diverse and are not included in this report.

Part 1 is organized to reflect the way in which grants augment and support the in-house program. Many of the grants relate to different parts of the in-house program, so each grant report is presented immediately following its related in-house priority project. They are arranged in eleven groups:

Carbon Monoxide Prediction
Soot Formation
Turbulent Combustion
Polymer Gasification
Toxic Potency
Furniture Flammability
Wall Fires
Fire Suppression
Fire Hazard Assessment
Engineering Analysis Systems
Large Fires

The projects for other agencies, presented in Part 2, although usually related to internally funded work, are primarily designed to meet the missions of those agencies and organizations. They are listed in two broad categories that complement the fire research program. They are:

Fire Science/Modeling
Fire Protection Technology

For the convenience of the reader, an alphabetical listing of all grants is contained in the Appendix.

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Part 1.0 Basic Research and Tools for "Engineered" Fire Safety (in-house projects and associated grants funded by NIST)

1.1 Carbon Monoxide Prediction

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - 1991

CARBON MONOXIDE PRODUCTION AND PREDICTION

Professional Personnel

William M. Pitts, Project Leader
Vytenis Babrauskas, Head, Fire Toxicity Measurement Group
Nelson P. Bryner, Chemical Engineer
Leonard Y. Cooper, Mechanical Engineer
Erik L. Johnsson, Mechanical Engineer
George W. Mulholland, Research Chemist
William J. Parker, Guest Worker
William H. Twilley, Engineering Technician

Project Objective

To provide the HAZARD team with an understanding of the mechanisms of carbon monoxide (CO) formation and sufficient algorithms to allow the development of tools which engineers and material designers can utilize to make accurate predictions of the quantity of CO produced under specified conditions.

Scope

This program is designed to assess the importance of CO in fire toxicology (i.e., the levels of CO generated) and to provide the scientific background required to allow the prediction of CO in real fires. Efforts range from purely empirical studies such as assessments of CO production in full-scale fire tests to fundamental studies designed to improve the understanding of the chemically reacting turbulent flows which ultimately produce CO. New information which is generated is incorporated into existing BFRL models of fire behavior.

Technical Accomplishments

During FY91 work has focused on four (discussed below) components of the overall priority project plan [see W. M. Pitts, "Long-Range Plan for a Research Project on Carbon Monoxide Production and Prediction," NISTIR 89-4185, October 1989]. All of these components are designed to assess whether or not the global equivalence ratio (GER) concept offers a viable approach for the prediction of CO formation in real fire situations. The GER concept refers to the experimental observation that concentrations of major gas species, including CO, in the well defined layers of combustion gases above simple fires can be correlated in terms of the GER. The GER is defined as the ratio of fuel to air available divided by the ratio of fuel and air required for complete combustion to water and carbon dioxide.

1. Investigation of CO Formation in a Reduced-Scale Enclosure (Bryner)

Despite the importance of the problem, very few detailed investigations of CO production during full-scale fire tests are available. The principal reason for this lack of data is the high cost associated with full-scale testing. An approach which is often used is to perform experiments on a reduced scale

where costs are lower and the tests are more easily manageable. A major drawback to this approach is that all the important fire parameters cannot be scaled simultaneously. Despite this, reduced-scale testing has contributed immensely to the understanding of fire behavior for conditions where the effects of scaling are properly understood. A reduced-scale enclosure (RSE) fabricated here at NIST is being used to characterize CO formation for a variety of test conditions using natural gas as fuel. Once an extensive data base is available, selected full-scale tests will be carried out to assess the effects of scaling.

Dimensional scaling has been used in the design of the RSE. The relative dimensions are based on those for the proposed ASTM Procedure "Proposed Method for Wall and Ceiling Materials and Assemblies" which includes a specification for a test room which is used in a number of laboratories for a variety of fire tests. The prescribed room is a 2.44 x 3.66 x 2.44 m^3 enclosure with a 0.76 x 2.03 m^2 doorway centered in one of the narrow walls. The RSE has dimensions corresponding to a 2/5 scale factor (i.e., 0.98 x 1.46 x 0.98 m^3). The doorway is scaled such that $Ah^{1/2} = 2/5$. This is the standard procedure for properly scaling enclosure ventilation. The RSE is designed in such a way that the wall containing the doorway can be replaced with ones having differently sized doorways. In this manner the ventilation factor for the room can be easily varied.

Instrumentation available for measurements includes CO, CO_2, and oxygen meters for measuring concentration of flame gases (dry basis) extracted from the enclosure, thermocouple trees for temperature measurement, and a pressure gage for recording the pressure within the enclosure. A total hydrocarbon analyzer has been ordered and will be installed in the system later in the year. RSE test burns are conducted under the furniture calorimeter. Measurements performed in the calorimeter include an oxygen depletion estimate of heat release rate as well as concentrations of CO, CO_2, and O_2 and smoke density.

During the past year over sixty tests have been made in the RSE using natural gas as fuel. The fuel flow rate, which is maintained constant throughout a given test, has been varied from fully ventilated to underventilated burning conditions. For fully ventilated cases very low levels of CO are generated. As the fuel flow rate is increased there is a rapid increase in the upper-layer CO concentration for global equivalence ratios near one. At the same time the concentration of oxygen in the layer drops to very low values. CO concentrations of several per cent are observed. Comparisons are currently being made with data generated by Morehart et al. (J. H. Morehart, E. E. Zukoski, and T. Kubota, NIST-GCR-90-585) for a simple flame system designed to investigate the dependence of CO generation on the GER. The results of this comparison will be used to assess the validity of the GER concept.

2. Chemical Stability of Upper Layers in Fires (Pitts)

A necessary condition for the GER concept to hold is that the layer of gases outside of and above the fire be nonreactive. For GER values less than 0.5 this is expected to be the case since very little fuel or products of incomplete combustion are present. As the GER becomes greater than ≈ 0.5 the upper-layer composition starts to change. Experiments indicate that in addition to CO_2 and water; unreacted fuel, a variety of hydrocarbons and soot, carbon monoxide, and hydrogen are found in upper layers in increasing amounts with increasing GER. For sufficiently high upper-layer temperatures, additional chemical reaction outside of the immediate flame zone is to be expected for these rich conditions.

During the past year the reactivity of these upper-layer gases has been investigated using full-kinetic calculations. For these calculations it has been assumed that only homogeneous (i.e. gas phase)

reactions are important. The role of heterogeneous reactions (e.g., those involving soot) will be the subject of a later study. Two limits of possible mixing behaviors--a perfectly stirred reactor (infinite mixing rate) and a plug flow reactor (no mixing)--have been treated. Full kinetic codes developed at Sandia National Laboratories were used for the calculations. The chemical mechanism used was that developed and validated by Dagaut et al. (P. Dagaut, J.-C. Boettner, and M. Cathonnet, Int. J. Chem. Kin. 22 (1990) 641-664) which includes 31 chemical species and 183 reactions.

Initial concentrations of flame gases are taken from the experimental findings of Morehart et al. Calculations have been made as a function of GER (0.5-2.8), residence time in the upper layer (0-20 s), and the temperature of the upper layer (700-1300 K). The results show that for temperatures below 800 K reaction is very slow. At higher temperatures the layer becomes reactive. As the temperature is increased the rate of reaction increases quickly. Reactions continue until either fuel or oxygen are depleted. For GER values less than one reaction is complete and CO_2 and water are generated. When GER values are greater than one significant amounts of CO are generated while the concentration of CO_2 is hardly modified. Interestingly, for rich conditions and temperatures below 1000 K the major products are CO and water. At higher temperatures more hydrogen is formed with the result that even higher levels of CO are observed since oxygen atoms which were tied up in water are available to form CO.

The GER concept is based on measurements of gas composition in hoods located above simple turbulent fires. Upper-layer temperatures in these experiments are generally less than 800 K. The calculations show that reaction should occur slowly for these condition. The temperatures observed in the upper layer of enclosure fires for underventilated conditions are generally in the 1200-1300 K range. The calculations indicate that upper-layer gas compositions observed in the experiments used to develop the GER concept become reactive at these temperatures. This suggests that great care should be used in extending the GER concept to room fire environments.

3. Development of a Mathematical Model for the Time Dependent Development of CO Concentration in an Enclosure (Cooper)

The experiments which have led to the development of the GER concept have all been steady state. Fires are dynamic events and the concentrations of flame gases in an upper layer are expected to change during the fire history. At early times the upper layer is likely to be lean, but as the fire grows and combustion products build up, the layer will become richer and richer with considerably higher concentrations of CO to be expected.

A general model, denoted as the generalized global equivalence ratio model (GGERM), has been developed to predict the generation rates of oxygen, fuel, and any other products of combustion in rooms containing fires. An algorithm for implementing the model has also been prepared. During the past year the model was exercised for a variety of fire conditions.

Some experimental data is available for testing the GGERM. Professor Roby and his students at VPISU have reported measurements of upper-layer gases for hexane burning in a compartment configured such that all air enters from the bottom and all combustion gases exit from a window. The upper-layer temperatures, air in-flow rates, and fuel burning rates have been measured. These are the parameters required to make predictions of the time development of upper-layer gas concentrations using the GGERM. Comparisons of experimental findings and predicted behaviors for hexane, oxygen, CO_2, H_2O, CO, and H_2 have been made. For those cases where experimental data are available the agreement is quite encouraging.

4. Development of an Instrument for Measuring the Global Equivalence Ratios in Fire Gases (Mulholland and Babrauskas)

It is obvious that the GER is an appropriate dependent variable for attempting to correlate measurements of CO concentration and production in enclosure fires. At the present time the techniques employed for GER measurements in earlier idealized laboratory investigations of underventilated burning cannot be implemented in our reduced- or full-scale experiments. As a result, there is a pressing need for an instrument capable of recording accurate GER values for gases extracted from the upper layer of a fire room. Such an instrument is currently being developed at NIST. This instrument is often referred to as the phi-meter (ϕ-meter).

The operating principle of the ϕ-meter is quite simple. Combustion products are extracted from the volume of interest and transported to the analyzer. Sufficient oxygen is added to the flow to insure complete conversion of all products to CO_2 and water. The gases then pass through a heated tube furnace where an appropriate catalyst is used to promote complete conversion. By measuring the oxygen concentration following passage through the converter and knowing the amount of oxygen added it is possible to calculate the GER.

Significant progress has been made in the development of the meter during the past year. An analysis was completed which showed the validity of the concept. A prototype instrument was then fabricated. The prototype was first tested by measuring the equivalence ratio for known flows (nonburning) of methane, O_2, and N_2. Excellent agreement between the ϕ values measured by the device and those derived from the known gas flow rates was found. Later measurements for the same fuel were done by extracting gas from the flow above a premixed burner. Over the range for which the methane/air mixtures were flammable the burner was ignited and the extracted gases were combustion products. For the other equivalence ratios no combustion occurred and the gases were simply extracted from the burner flow. Again, excellent agreement between the nominal equivalence ratio and the measured values was obtained. Testing and development is continuing.

Reports and Publications

"The Effect of Oxygen Concentration on CO and Smoke Produced by Flames," G. Mulholland, M. Janssens, S. Yusa, W. Twilley, and V. Babrauskas, Paper presented at the 3rd International Symposium on Fire Safety Science, July, 1991. (to be published)

"A Model for Predicting the Generation Rate and Distribution of Products of Combustion in Two-Layer Fire Environments," L. Y. Cooper, National Institute of Standards and Technology Internal Report, NISTIR 90-4403, October, 1990.

"Application of the Generalized Equivalence Ratio Model (GGERM) for Predicting the Generation Rate and Distribution of Products of Combustion in Two-Layer Fire Environments--Methane and Hexanes", L. Y. Cooper, National Institute of Standards and Technology Internal Report, NISTIR 4590, June, 1991.

Related Grants

"Fundamental Mechanisms for CO and Soot Formation in Diffusion Flames," Robert J. Santoro, Pennsylvania State University.

"Radiation From Turbulent Luminous Fires," Gerard M. Faeth, University of Michigan.

"Experimental Study of the Environment and Heat Transfer in a Room Fire," Edward E. Zukoski, California Institute of Technology.

"Compartment Fire Combustion Dynamics," Richard J. Roby, Virginia Polytechnic Institute and State University and C. L. Beyler, Hughes Associates.

"Simplification of Diffusion Flame Chemistry: A Theoretical and Experimental Study of the Structure of Laminar Diffusion Flames," J. Houston Miller, George Washington University.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution: Virginia Polytechnic Institute & State University
Grant No.: 60NANB8D0829
Grant Title: Compartment Fire Combustion Dynamics
Principal Investigators: Richard J. Roby
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NIST Scientific Officer: Dr. William M. Pitts

Technical Abstract:

In a typical compartment fire a two layer system is created in which the upper layer consists of the products of combustion and the lower layer consists of primarily ambient air which is convectively heated prior to plume entrainment. As the fire progresses, the upper layer will grow and the layer interface will move toward the floor. The upper layer will spill into adjacent hallways or rooms as the layer interface descends below the top of doorways or other openings. Life threatening concentrations of CO and smoke arise when the flow dynamics create underventilated conditions in the upper layer. This study is directed toward understanding the generation and spread of toxic gases, particularly carbon monoxide, in realistic compartment fires.

The three year research effort is designed to experimentally 1) determine the effects of realistic fire flows on species generation rates and their correlation with equivalence ratio, 2) establish major toxic gas and smoke generation rates for important fuels such as PMMA, wood and TDI-based polyurethane, and 3) determine the efficiency of external flames in destroying major toxic gases produced within the compartment during oxygen deficient combustion.

The test apparatus used for this investigation is a two level structure consisting of a 1.2 m x 1.5 m x 1.2 m fire compartment with 2.54 cm thick Fire Master, UL rated, fire insulation board completely covering the interior surfaces and a 1.2 m x 1.4 m x .3 m high air distribution plenum below this box. The compartment has two ventilation paths. A lower opening allows air to be naturally drawn into the compartment through a 4 m long 30.5 cm diameter inlet duct which empties into the distribution plenum. The air in the plenum is uniformly drawn into the lower section of the fire compartment through thermally shielded vents on each side of the structure. A window style exhaust vent is horizontally centered in the front of the compartment. The vent size was varied to produce different ventilation conditions while also assuring that there was only outflow of combustion products. A 1.5 x 1.5 m hood positioned over the exhaust vent collects all fire effluent. The hood is exhausted through 45.7 cm duct fitted with a probe and orifice plate to allow for downstream sampling of the fire effluent and measurement of the volumetric duct

flow. A smoke measurement device is situated downstream of the sampling probe and upstream of the orifice plate. The smoke measurement device provides extinction coefficients by measuring the attenuation of a 670 nm laser beam passed through the exhaust duct. From the extinction coefficient the smoke volume fraction [1] and the smoke yield [2] can be formulated. The overall fuel-to-air ratio of the compartment was obtained by measuring the fuel volatilization rate by use of a load cell and by measuring the air flow rate in the inlet duct by use of a linear velocity probe. CO, CO_2 and O_2 concentrations were measured continuously by probe sampling, and temperature measurements were made from a vertical tree of eight aspirated thermocouples located in the front corner of the compartment.

The fuels investigated were chosen to provide a varied selection in order to see if correlations obtained were independent of fuel type. Hexane was chosen as a simple liquid fuel which had been studied previously by Beyler in a hood environment [1,2]. PMMA was then selected as a simple to analyze complex hydrocarbon since it breaks down almost entirely to its monomer as it volatilizes. TDI-based Polyurethane, however, is a more complex polymer that does not decompose to simple monomers. Spruce represents a cellulosic material that decomposes directly from a solid to volatiles and char. Besides being complex fuels, polyurethane and wood are common materials used in buildings and furnishings.

Several general observations have been made that show the strong dependance of compartment fire characteristics on transition from overventilated (equivalence ratio less than one) to underventilated conditions. The plume equivalence ratio is the ratio of fuel volatilization rate to air entrainment rate normalized by the stoichiometric fuel to air ratio. In general, negligible CO concentrations (less than 0.1%) exist until the overall equivalence ratio reaches a value near one for all fuels. As the compartment becomes underventilated the CO concentration rises sharply reaching lethal levels and the O_2 concentration decreases rapidly to below life sustaining conditions. Also, external burning and external flame jets do not occur unless underventilated conditions exist.

The experiments show repeatable correlations between species yields and plume equivalence ratio. Yield is the grams of species produced per gram of fuel burned. The correlations between steady-state normalized CO yields and overall equivalence ratio for the four fuels are shown in Figure 1. The yields are normalized by the maximum possible yield of CO for the respective fuel. Up to an equivalence ratio of 1, there is negligible CO yield. At equivalence ratios greater than 1.5 a leveling off of CO yield is observed at approximately 0.12.

The higher CO yields for the polyurethane are believed to be due to the conversion of CO to CO_2 freezing out. Chemical kinetic modeling suggests that the freeze out temperature is about 875 K. Most of the polyurethane fires have average upper layer temperatures below this freeze out point. Normalized CO_2 yield correlations collapse down to one curve for all four fuels, Figure 2. The lower wood and polyurethane yields between an equivalence ratio of 0.4 and 1 are again attributed to the low upper layer temperatures (below 875 K) that favor the production of CO over CO_2.

As fuel rich gases spill into adjacent areas, ambient air can be entrained resulting in ignition and burning outside of the main compartment fire. Little known work has been done on the effect of external burning on CO and smoke yield. Arguments can be made that CO yield increases due to external burning because unburned fuel in the spilled upper layer is burned and the reactions are quickly quenched leaving a higher yield of CO then what was present in the compartment upper layer. On the other hand, CO yield may be reduced as CO and unburned hydrocarbons both burn to completion.

The effect of external burning on CO and smoke yields from compartment fires was investigated. A window-style exhaust vent was used for the external burning experiments and species yields were measured in the exhaust duct downstream of the compartment. The yields measured downstream of the exhaust vent were compared to yields measured in the compartment upper layer for similar hexane-fueled fires, see Figure 3. External burning of fuel

rich exhaust gases significantly reduces the CO yield to below life threatening levels. The exhaust-sampled fires with steady-state, average plume equivalence ratios greater than 2 were always observed to have sustained external burning, whereas, the fires with equivalence ratios below 2 had no sustained external burning.

Smoke volume fraction measurements show that smoke decreased with the occurrence of external burning. As can be seen in figure 4, time histories during a fire show that the smoke volume fraction curve is qualitatively the same as the CO concentration curve. The drop in CO and smoke between 280 s and 320 s corresponds to the time in which external burning was present. The dramatic decrease in CO yield and smoke and the fact that the CO_2 yield approximately reaches a maximum indicates that very nearly all carbon in CO and soot in the upper layer is converted to CO_2 when external burning occurs. Smoke volume fractions of 1 to 3 ppm were observed for the hexane fires. The smoke volume fraction for wood fires was below 0.5 ppm at equivalence ratios below 1 and ranged from 1 to 2 ppm for equivalence ratios from 1 to 2.2. Polyurethane fires had smoke volume fractions ranging from 0.8 ppm at an equivalence ratio of 0.35 to 6 ppm at an equivalence ratio of 2.

Utilization of Results:

This project provides direct support to the development of toxic hazard analysis techniques by providing basic data for the modeling of toxic gas production. In addition, through the experiments involving external flames, it provides information about the spread of toxic species from the compartment of fire origin. Since the spread of toxic gases is frequently involved in fire deaths remote from the compartment of origin, this data is crucial to modeling the overall fire hazard in a building. The development of these models and this data will markedly improve the ability to assess the impact of different building materials and building designs on the fire safety provided.

Papers:

Gottuk, D. T., Roby, R. J. and C. L. Beyler, "Carbon Monoxide Formation in Hexane-Fueled Compartment Fires," Poster presented at the Twenty-Third International Symposium on Combustion, Orleans, France, July 1990.

Gottuk, D. T., Roby, R. J. and C. L. Beyler, "Carbon Monoxide Yields from Hexane-Fueled Compartment Fires," paper no. 65, presented at the Eastern States Section Meeting of the Combustion Institute, Orlando, FL, December, 1990.

Skelly, M. J., R. J. Roby, and C. L. Beyler, "An Experimental Investigation of Window Breakage in Compartment Fires," Journal of Fire Protection Engineering, 3(1),1991 pp 25-34.

Gottuk, D. T., Roby, R. J. and C. L. Beyler, "Carbon Monoxide Formation in Hexane and PMMA-Fueled Compartment Fires," Poster presented at the Third International Symposium on Fire Safety Science, Edinburgh, Scotland, July 1991.

Gottuk, D. T., Roby, R. J. and C. L. Beyler, "The Effect of External Burning on Carbon Monoxide and Smoke Yields from Hexane-Fueled Compartment Fires," submitted for presentation at the Eastern States Section Meeting of the Combustion Institute, Ithaca, NY, 1991.

Gottuk, D. T., Roby, R. J. and C. L. Beyler, "Effect of Temperature on Species Yields in Compartment Fires," in preparation for journal submission.

Gottuk, D. T., Roby, R. J. and C. L. Beyler, "The Study of Four Fuels in a Compartment Fire Apparatus with Direct Measurement of the Air Entrainment Rate," in preparation for journal submission.

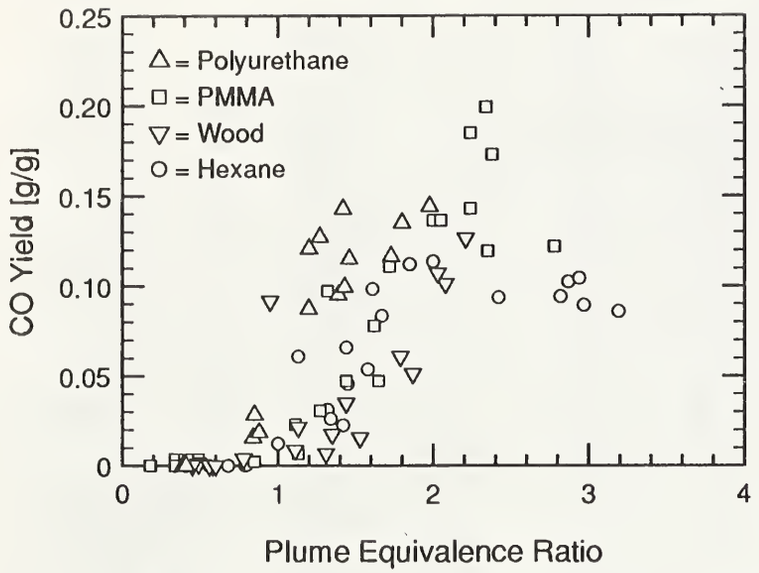

Figure 1. Normalized CO Yield Correlations

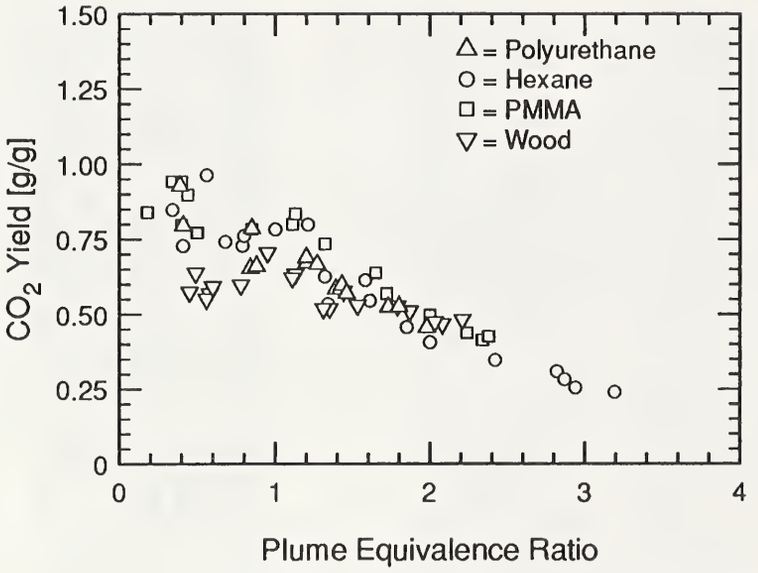

Figure 2. Normalized CO_2 Yield Correlations

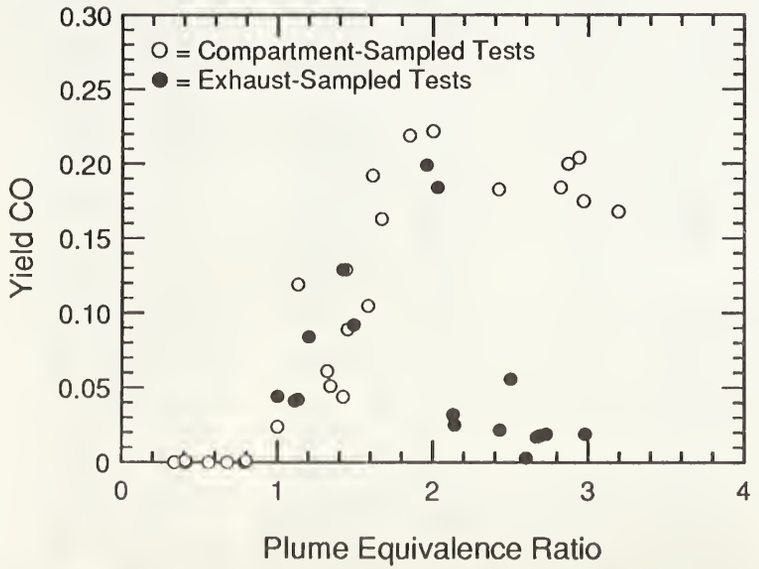

Figure 3. Hexane CO Yield Correlation with External Burning

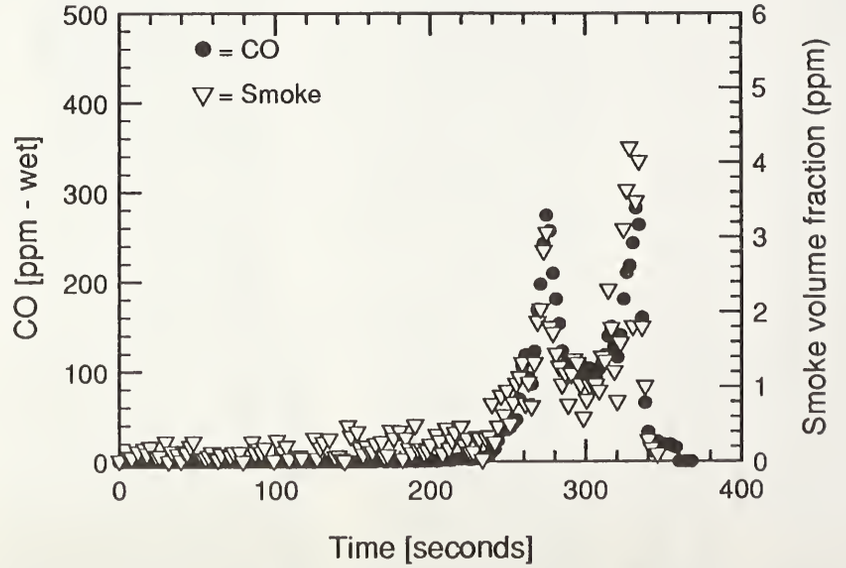

Figure 4. CO and Smoke Generation During a Hexane Fire with External Burning

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution: California Institute of Technology

Grant Number: 60NANB9D0958

Grant Title: Experimental Study of Heat Transfer and the Environment in a Room Fire

Principal Investigator: E. E. Zukoski
Jet Propulsion Center, 301-46
California Institute of Technology
Pasadena, CA 91125

Other Professional Personnel: T. Kubota, Professor Emeritus
R. Chan, Doctoral Student
R. McGuffin, Doctoral Student

NIST Scientific Officer: Dr. Leonard Y. Cooper

TECHNICAL ABSTRACT:

INTRODUCTION The characteristics of large diffusion flames burning in a vitiated atmosphere and the flow of gravity currents in hallways are under investigation in two experimental programs.

The composition of the gas surrounding a large diffusion flame has a strong effect on the chemical species formed during the combustion process and a surprisingly weak influence on the flame height. We are studying these properties of large diffusion flames under two conditions: In the first, the flame penetrates far above the interface between a cool lower layer of fresh air and a strongly vitiated the upper layer, and the emphasis in this study is to measure the products formed during the transient development of the upper layer. In the second condition, the flame is entirely within an atmosphere vitiated by combustion, and we have been interested in studying the species produced and the geometry of the flame as the oxygen mass fraction is reduced to the flame extinction condition.

The second area of interest concerns an investigation of the influence of viscosity on the flow in a gravity current such as that which would develop in a long hall during an accidental fire. The study has made use of the salt-water/water modeling of these currents in order to separate the influences of heat transfer and viscosity on the development of the currents in long halls. The two papers listed in the References section discuss in greater detail some of the results presented here.

CHARACTERISTICS OF LARGE DIFFUSION FLAMES The flame length and chemical species produced in diffusion flames of natural gas stabilized on 20- and 50-cm diameter porous bed burners are being studied for several conditions of the ambient gas which surrounds the burner.

These experiments are being carried out in a hood which is a 1.83-m cube and a gas

chromatograph is being used to study the chemical species produced in the flame. On-line infrared systems are also being used to obtain a continuous measure of the mole fractions of carbon monoxide and carbon dioxide. In addition to studying the effect on flame length of the reduction in mole fraction of oxygen in the ambient gas we have also determined the influence of nitrogen addition to the fuel on the flame length of natural gas flames burning in air.

The dependence of flame length on oxygen mass fraction in the ambient air is shown in Figure 1 for a 13.6-kW natural gas flame stabilized on a 20-cm diameter porous bed burner. In these experiments, the oxygen mass fraction was reduced by addition of products of composition to the gas within the hood. The flame length reported here was obtained by taking video pictures of the flame at 30 frames per second, measuring the flame height in each photograph, and then finding the 50% intermittency length from several hundred frames.

The data clearly show that the flame length increases by less than 10% as the oxygen concentration is reduced from a value corresponding to pure air to values close to the flammability limit where soot production has completely stopped. This data and that obtained for other flames stabilized on 20-cm and 50-cm burners show a similar trend.

Some of the data of Figure 1 are cross plotted versus the ambient gas temperature in Figure 2 to show that the increase in flame length is not caused by the temperature changes which accompany the vitiation of the gas surrounding the flame. For example, the data for 17% mole fraction of oxygen, shown in Figure 2, cover a large part of the temperature range obtained in these tests but show no systematic dependence on ambient temperature.

Similarly, the adding nitrogen to a constant flow of natural gas was found to have a very small influence on flame length. A typical data set is shown in Figure 3 for a 43-KW natural gas fire stabilized on a 50-cm burner. In these experiments, the total heat release was kept constant by holding the flow rate of natural gas fixed; the addition of nitrogen gas to the fuel flow produced a "fuel gas" in which the heating value was decreased by a factor of more than 6.

If we assume that the flame length depends only on the Q^* parameter, which we have used as a correlating parameter for flame length in the past, both of these results appear to be rational. However, the weak dependence of flame length on both the oxygen mass fraction and on the high concentration of nitrogen gas in the fuel is surprising to this author. The lack of dependence on oxygen concentration is particularly troublesome and has interesting implications concerning entrainment and combustion in large diffusion flames.

SPECIES PRODUCED DURING THE DEVELOPMENT OF A CEILING LAYER In these experiments, we are measuring the species produced during the development of the ceiling layer by a natural gas fire with a fixed heat fuel flow rate. In particular we are measuring the mole fraction of carbon dioxide and monoxide during the development of the ceiling layer in a hood with is a 1.83-m cube. Continuous measurements of the concentrations of CO and CO_2 are made and the temperature and other species are measured at various intervals to allow the comparison of the data with modeling results.

The fire is started with the burner located a the selected elevation beneath the hood, and temperature and species are measured as the composition of the gas within the hood approaches a steady value. For heat release rates of 20 kW, the time required is of the order of 10 minutes. Preliminary measurements have been completed, and several definitive sets of data are being obtained.

GRAVITY CURRENTS A report on our gravity current experiments and a computational model for the current are being completed. With the aid of Dr. Kubota, we

have finally developed a computational method which will allow us to develop an analytic model for the gravity current which includes viscous effects.

In the inviscid case, the predicted properties of the gravity current and the wave reflected from the closed end of the hall agree with our expectations and the model is now being extended to include viscous effects. Eventually, we expect to be able to include the effects of heat transfer as well as viscosity in this calculation.

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FIGURES

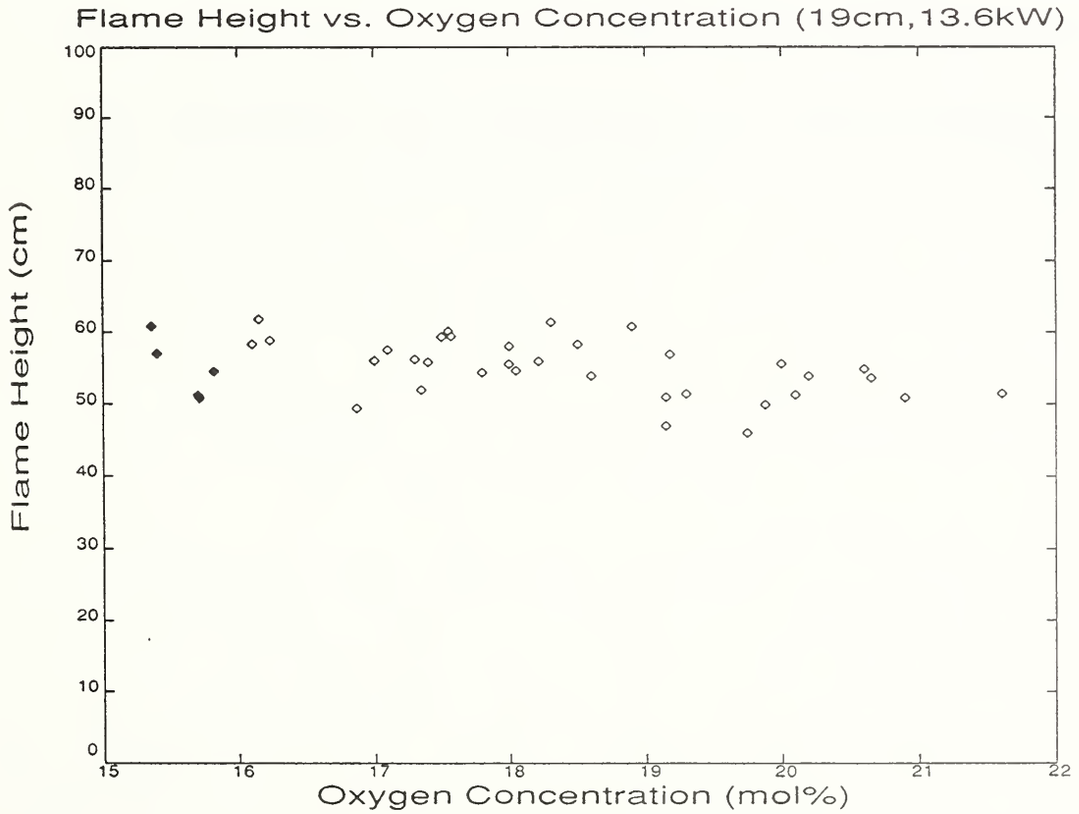

Figure 1.

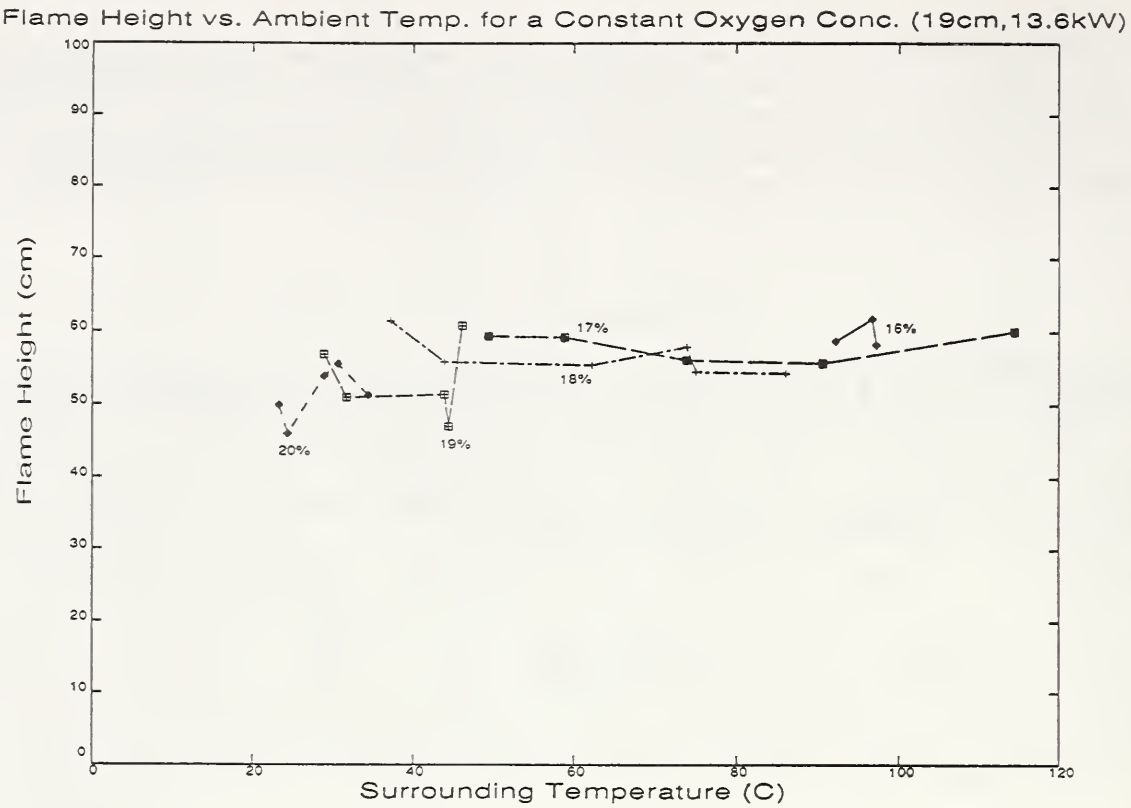

Figure 2.

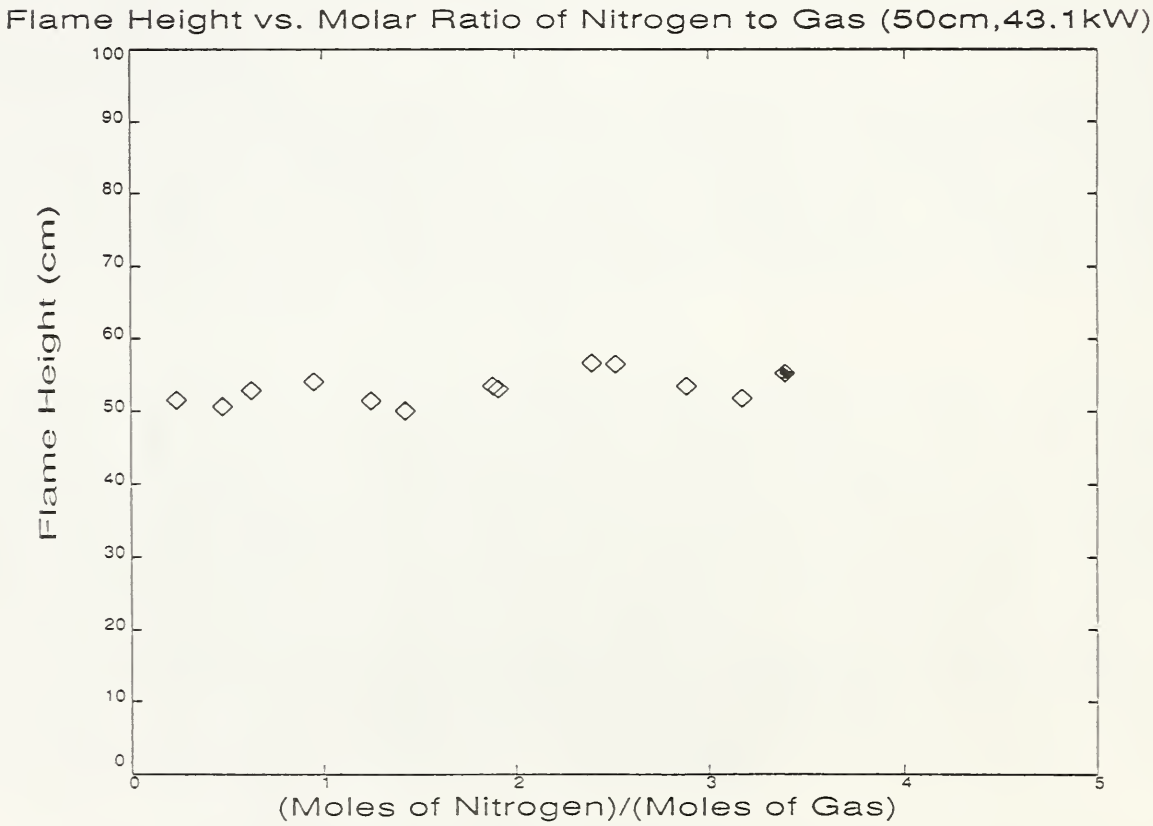

Figure 3.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 91

Institution: The Pennsylvania State University

Grant No.: 60NANB01035

Grant Title: Fundamental Mechanisms of CO and Soot Formation in Diffusion Flames

Principal Investigator: Professor Robert J. Santoro
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University Park, PA 16802

Other Professional Personnel: T. F. Richardson, Doctoral Student
R. Puri, Doctoral Student
M. Moser, Doctoral Student

NIST Scientific Officer: Dr. Kermit C. Smyth

Technical Abstract:

Introduction. Carbon monoxide and soot represent the most serious combustion products formed in fires with respect to loss of life and injury. Consequently, an understanding of processes which control their formation and destruction is critical to fire modeling and impact mitigation. The high concentrations of CO and soot that characterize typical fire situations are recognized to be interrelated. The fundamental nature of this interaction is being investigated in this study. Two possible mechanisms that could affect the concentration of CO in the presence of soot, namely radiative quenching and competition for oxidizer species, are being examined. In the past, equilibrium estimates of OH concentration have been used to determine that radiative quenching can account for the higher CO observed in the fuel lean regions of diffusion flames [1]. The soot oxidation rates, based on surface area evaluated from optical measurements alone, allowed the inference that competition between CO and soot for OH in both fuel lean and fuel rich regions of the flame could also contribute to the higher CO emissions [1]. However, uncertainties in the soot surface area and the OH reaction efficiency with soot precluded a quantitative evaluation of the relative importance of these two mechanisms. Therefore recent efforts have focussed on measuring the OH concentration and improving estimates of soot surface area using Transmission Electron Microscope (TEM) measurements of primary particle size.

OH Measurements. Laser-induced fluorescence (LIF) was utilized to measure OH concentrations in a series of methane and ethene laminar diffusion flames burning in air. The burner, which is coannular in geometry, has been extensively described [2]. It consists of a 1.11 cm fuel tube surrounded by a 10.18 cm air annulus. Both methane and ethene fuels were studied at volumetric flow rates corresponding to 7.7 cm^3/s for methane and 3.85, 4.6 and 4.9 cm^3/s for ethene. The air flow rate for the methane flame and the 3.85 cm^3/s ethene flame was 1062 cm^3/s and, for the higher ethene flow rate flames was 1298 cm^3/s. For the ethene flame having the lowest fuel flow rate, no soot is observed to survive the flame tip, while for the largest fuel flow rate case soot is clearly observed to issue from the flame. For the 4.6 cm^3/s flow rate, the flame is quite close to the smoke point condition [3]. In addition to the coannular flame measurements, profile measurements were made in a Wolfhard-Parker flame using methane as the fuel. These studies were carried out to provide a comparative basis from which to determine the absolute OH concentration in the coannular flames.

The LIF measurements were made using a Nd:YAG pumped dye laser whose output was frequency doubled to produce light at 278.83 nm and 283.55 nm. These wavelengths excite the $S_{21}(8)$ and the $Q_1(8)$ lines of the $A^2\Sigma^+ \leftarrow X^2\Pi_i$ (1,0) band of OH respectively and were selected to minimize the variation of the rotational population level with temperature. Fluorescence was measured at 90° using longpass glass

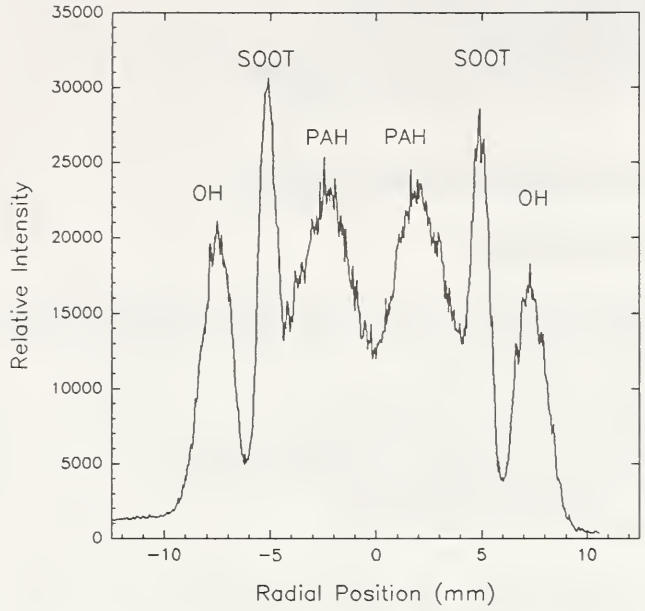

Figure 1. Laser-Induced Fluorescence in the axisymmetric ethene flame (Fuel flow rate = 3.85 cm^3/s, H = 7 mm).

filters which minimized elastically scattered light while transmitting the (0,0) band emission of OH at 308 nm.

In order to calibrate the peak OH concentration in the coannular burner the following steps were taken. First, point profile measurements were made in a methane-air flame stabilized on the rectangular slot (Wolfhard-Parker) burner, where previous absorption measurements have established the peak OH concentration [4]. Next, LIF signal levels in the methane-air flame on the rectangular slot burner were compared with those from the methane-air flame on the axisymmetric burner. Point profile measurements were also made in the ethene flame with the lowest flow rate.

For the fluorescence measurements in the coannular burner, light detection was accomplished using a cooled CCD detector with camera control and data storage with a 386 personal computer. Both 1D line and 2D planar images of the resulting fluorescence were recorded. The 1D line images were obtained by exciting the $S_{21}(8)$ OH line, while the 2D planar images were obtained by exciting the stronger $Q_1(8)$ OH line. The results presented here are raw signals and need to be corrected for the variations in laser pulse energy and the local quenching rate.

An example of a typical fluorescence profile is shown in Figure 1. Three distinct contributions are observed from OH, soot and polynuclear aromatic hydrocarbon (PAH) species [5]. When the laser was tuned off resonance with respect to the OH rotational line, the two peaks furthest from the burner centerline disappeared, while the features attributed to soot scattering and PAH fluorescence remained.

Figure 2 shows a series of OH fluorescence intensity profiles for several axial positions in the methane flame. The soot and PAH signals have been eliminated by subtracting the off resonance profile from the on resonance profile at each axial location. These results show a clear trend in the concentration profiles. The relative intensity decreases in magnitude and increases in spatial extent with height in the flame. The results for the ethene flame having a fuel flow rate of 3.85 cm^3/s show similar trends. It should be noted that the ethene flame has nearly an order of magnitude more soot than the methane flame.

The OH concentrations are difficult to determine in the soot region at higher heights in the ethene flames with higher fuel flow rates (and consequently higher soot concentrations). This is due to problems associated with the subtraction of two large soot signals relative to a much smaller OH signal. The 2D planar data were obtained using a stronger $Q_1(8)$ line and thus showed much larger OH signals relative to the soot scattering signals. Figure 3 presents the profiles obtained with the laser tuned both on and off resonance for the ethene sooting flame at a height of 100 mm. OH is present throughout the region where soot breaks out of the flame. Figure 4 shows the net OH signal obtained by subtracting the off resonance profile from the on resonance profile. Thus these results demonstrate the capability to measure OH concentration variations in the region of the diffusion flame tip where soot and CO oxidative steps compete for OH.

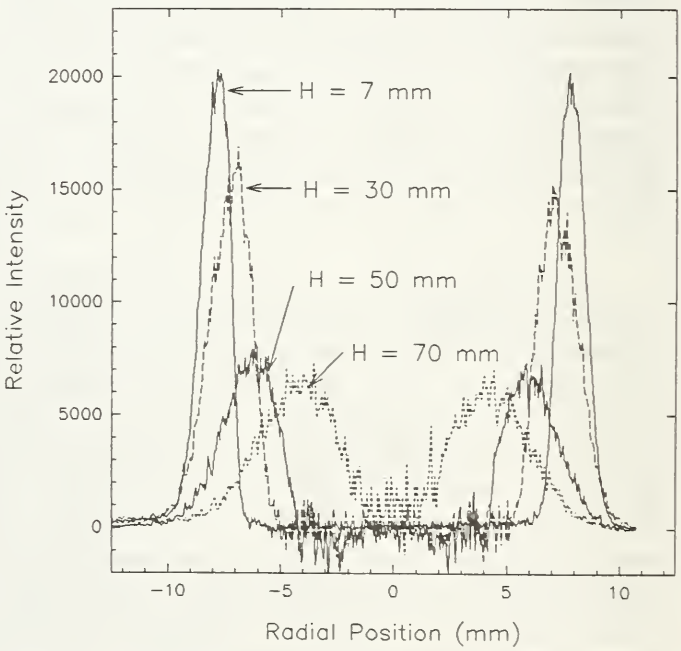

Figure 2. OH intensity profiles in the methane flame. Visible flame height = 79 mm.

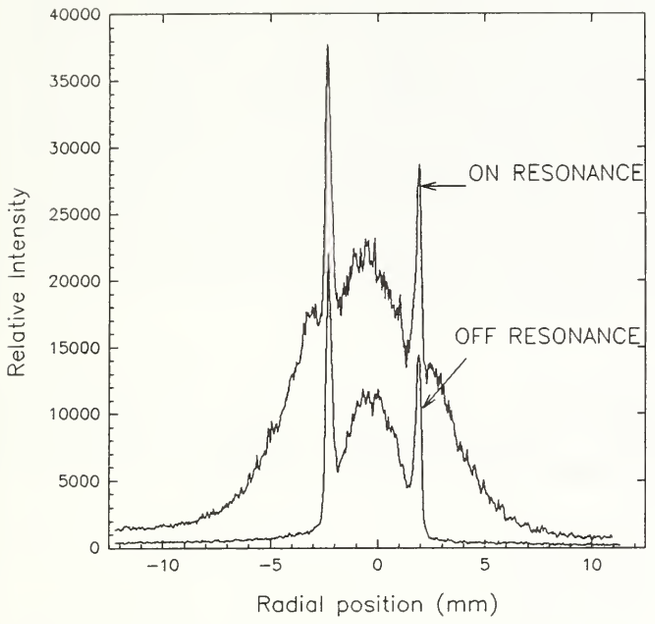

Figure 3. On and off resonance profiles for the sooting ethene flame (Fuel flow rate = 4.9 cm^3/s, H = 100 mm).

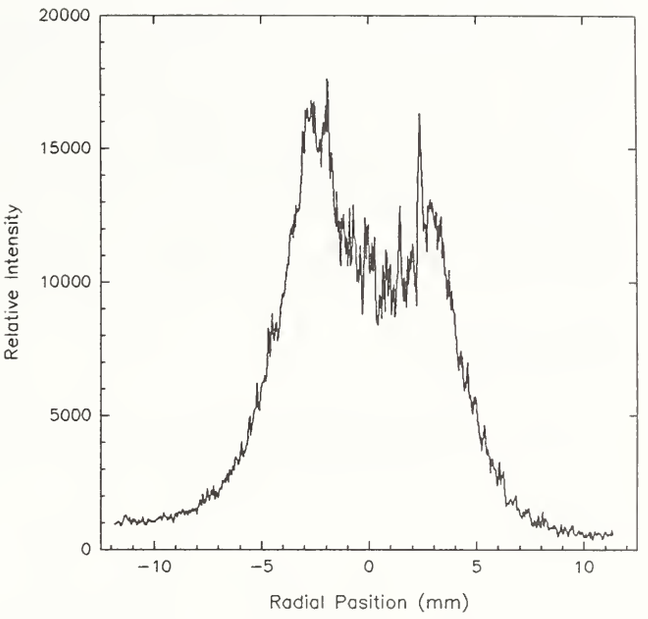

Figure 4. OH profile in the soot emitting ethene flame at H = 100mm.

TEM Measurements. The optical measurements of soot assume spherical particles and do not accommodate their aggregate nature. Consequently soot oxidation rates based on these measurements alone can be significantly in error. Thermophoretic sampling of soot aggregates on TEM grids yields primary particle size information, d_p, which, in combination with optical measurement of volume fraction, f_v, can give more accurate soot oxidation rates.

Thermophoretic sampling takes advantage of soot particle transport to a cold surface in the presence of a temperature gradient [6]. The thermophoretic probe consists of a carbon coated 200 mesh copper grid held in place between two strips of sheet metal, machined to expose the grid to the flame. The probe is rapidly located in the flame environment, exposing the grid to the soot field for 50 msec. This short exposure time provides a cold surface to quench the heterogeneous reactions on the captured particles. The TEM negatives at a magnification of 60K were imaged with a CID camera and the image analysis software was used to measure the primary particle sizes.

Figure 5 shows the temporal variation of primary particle size, d_p, along the centerline of a flame burning a mixture of methane and 1-butene. This flame, like the highest ethene flow flame, emits soot. The primary particle diameters shown in Figure 5 are arithmetic averages of 100 measurements or more at each temporal location. Since the measurements were made along a streamline, the number of primary particles, N_p, can be expected to be constant [7]. This intuitive observation can be exercised as a useful consistency check of the d_p and f_v measurements. This consistency check is currently in progress and soot oxidation rates based on these measurements will be forthcoming.

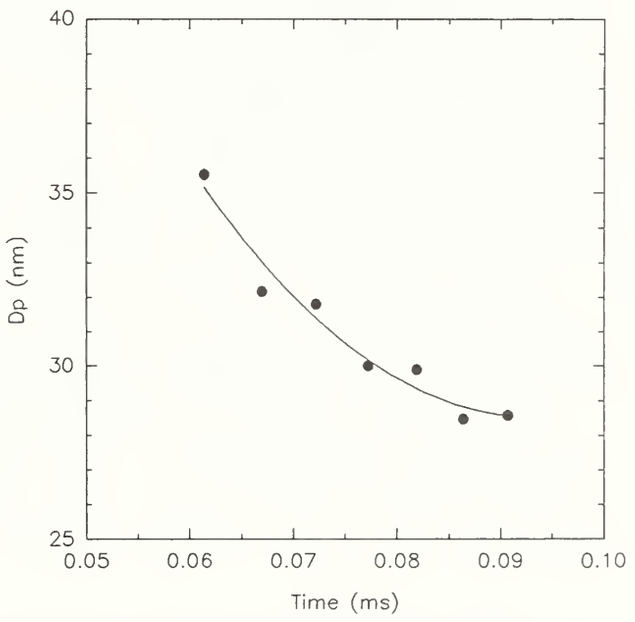

Figure 5. Temporal profile of the primary particle size, d_p, in the methane/1-butene flame.

Summary. One of the major objectives of the current study is to provide a quantitative basis from which to assess the competition between CO and

soot for OH species. In particular, it is desired to estimate the degree to which temperature reductions due to increased radiation from soot as compared to soot oxidation by OH are responsible for the higher levels of CO observed as the soot concentration increases [1]. Consequently, the OH concentration variation near the tip of the flame has been examined for non-soot emitting, near soot emitting and soot emitting conditions. Once the relative intensity profiles are converted to absolute OH concentrations and the TEM observations are checked for consistency, the previously measured soot volume fraction, CO, velocity and temperature fields can be used to evaluate the relative contributions of the temperature and reactive competitive mechanisms to the CO emissions observed for flames with increased soot loading. Based on these results, the fundamental mechanisms important in the formation and destruction of CO with respect to soot in fires can be incorporated into current fire models.

Acknowledgement

The hydroxyl radical measurements were obtained in collaboration with Dr. Kermit C. Smyth of the Building and Fire Research Laboratory and his contributions are gratefully acknowledged.

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BUILDING AND FIRE RESEARCH LABORATORY

FIRE RESEARCH PROGRAM

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

FY 91

Institution:	The University of Michigan
Grant No.:	60NANB8D0833
Grant Title:	Radiation from Turbulent Luminous Flames
Principal Investigator:	Professor G.M. Faeth Department of Aerospace Engineering 218 Aerospace Engineering Building The University of Michigan Ann Arbor, MI 48109-2140
Other Professional Personnel:	Ö.Ü. Köylü, Doctoral Candidate
NIST Scientific Officer:	Dr. Howard R. Baum

Technical Abstract:

Introduction. This investigation is considering three aspects of unwanted fires: (1) the relationship between CO and soot emissions, (2) the physical properties of soot emissions, and (3) the effects of turbulence/radiation interactions. Work on the last phase was limited to apparatus development so only the first two phases will be considered here. The findings have application to modeling fires in structures, developing materials test codes, and developing fire detectors.

CO and Soot Emissions. Carbon monoxide and soot are major hazards of fires: inhalation of carbon monoxide is the main cause of fatalities while soot obscures fire fighting efforts and increases flame spread and burning rates by increasing flame radiation. Additionally, many workers have noted a relationship between carbon monoxide and soot emissions from flames which indicates a synergism of these fire hazards. Thus, the objectives of this phase of the investigation are to study the emission of carbon monoxide and soot from overventilated buoyant turbulent diffusion flames, and to examine relationships between these two emissions. A wide range of gaseous and liquid fuel types was considered (alkynes, alkenes, alkanes, aromatics and alcohols) yielding fuel H/C ratios (atomic) in the range 1-2.67.

Experiments for the gaseous fuels involved burners having diameters of 5, 50 and 234mm; the liquid fuels involved burning from round wicks having diameters of 50, 125 and 195mm. Combustion was in still air with flame conditions ranging from buoyant jet flames to pool-like fires. The fuel-lean far-overfire region of the flames was observed using sampling and analysis by NDIR and gas chromatography to find CO concentrations and mixture fractions, and laser extinction at 632.8nm and analysis assuming the small-particle (Rayleigh) scattering limit to find soot volume fractions. Soot volumes were converted to soot mass assuming a soot density of 1100 kg/m^3.

It was found that variations of CO and soot concentrations in the overfire region of any given flame were consistent with passive mixing, and with CO concentrations, soot

concentrations, and mixture fractions, being relatively constant when chemical reactions are quenched near the flame sheet. The last observation is surprising because it is expected that regions near the base of the flame would have shorter residence times than near the flame tip, yielding different outcomes of the finite rate chemistry responsible for emissions of CO and soot. Based on this finding, it was possible to find CO and soot generation factors (defined as the mass of CO and soot emitted per unit mass of fuel carbon burned) that were essentially constant within the overfire region of a given flame.

The carbon monoxide and soot generation factors also were examined as a function of flame residence time, defined as the time between termination of the fuel flow rate and the disappearance of all flame luminosity. It was found that the generation factors varied at short residence times but became independent of residence time for residence times roughly an order of magnitude longer than the laminar smoke point residence time. Thus, within this long residence time regime, the generation factors are only functions of fuel type. This vastly simplifies characterization of CO and soot concentrations in the overfire region of turbulent flames in the long residence time regime that is most relevant for practical fires.

The relationship between CO and soot emissions can be seen from Fig. 1, which is a plot of CO generation factors for all the fuels. The results for each fuel are averaged over all residence times but the data base is dominated by the long residence time regime. CO generation factors for ethanol, methanol and methane are shown at the left of the plot to provide a baseline for nonsooting fuels. The measurements include present findings as well as earlier FMRC results reported by Tewarson (which are probably in the long residence time regime). The correlation between CO and soot emissions is striking, highlighting the synergism between these hazards. The results indicate that 0.37 kg of CO is produced for every kg of soot produced for heavily sooting fuels.

Results in Fig. 1 suggest the presence of sooting and nonsooting mechanisms of CO emissions from flames. The sooting mechanism appears to involve processes within the soot layer as it passes from fuel-rich to fuel-lean conditions near the tips of turbulent flamelets. This is plausible because the oxidation of soot yields CO as a first step so that the presence of soot implies the continued presence of CO. The nonsooting mechanism probably involves quenching of CO reactions as it diffuses away from the sides of turbulent flamelets toward fuel lean conditions — a conventional process reasonable for emission of other gaseous pollutants, like NOX, from flames. Nevertheless, the sooting mechanism of CO emissions is generally dominant for sooting overventilated flames.

Soot Physical Properties. Current work on flame emissions properties is focussed on the physical properties of soot in the overfire region of turbulent flames in the long residence time regime. These conditions are of interest to gain a better understanding of why soot generation factors become constant at long residence times. The results also are being used, in conjunction with approximate theory of soot aggregate optical properties, to evaluate earlier soot concentration measurements based on the small-particle (Rayleigh) scattering approximation.

The experiments involve thermophoretic sampling and TEM analysis of soot aggregates from various points in the overfire region and residence times (in the long residence time regime). All the sooting fuels discussed earlier were studied. It was found that the statistical properties of the soot aggregates varied with fuel type but were independent of position in the overfire region and flame residence time. This vastly simplifies characterization of overfire soot for practical turbulent flames to a single statistical population for each fuel.

Both primary particle diameter, d_p, and the number of primary particles per aggregate, N, satisfied log normal probability density functions. However, d_p had a relatively small variance yielding nearly monodisperse primary particle sizes while the standard deviation of N was larger than its mean value yielding a broad range of aggregate sizes, e.g., 95% of the aggregates

contained between 30 and 1800 primary particles. The aggregates exhibited mass fractal properties extending to aggregates of only a few particles.

The variation of aggregate structure properties with fuel type could be scaled roughly by the laminar smoke point residence time. The resulting correlations are illustrated in Fig. 2, considering mean primary particle diameter, $\bar{d}p$, geometric mean number of primary particles per aggregate, N_g, the moment ratio, $fn = \bar{N}^2/(\bar{N})^2$, and the mass fractal dimension, D_f. Within experimental uncertainties, only $\bar{d}p$ varies significantly, increasing from 30 to 51nm as the sooting tendency of the fuel increases. Based on soot concentrations measured earlier, rates of coalescence are negligible in the overfire region so the properties shown in Fig. 2 are invariant.

The soot structure measurements were used to compute aggregate optical properties from the approximate theory of Dobbins and coworkers. The mean ratio of scattering to absorption crossections, $\bar{\rho}_{sa}$, multiplied by the refractive index function, E(m)/F(m), is plotted as a function of wavelength, λ, in Fig. 3 for all the fuels. The results indicate large departures from Rayleigh scattering, $\bar{\rho}_{sa}$ significantly greater than zero, in the visible — particularly for heavily sooting fuels. However a number of aspects of the approximate theory are questionable — assumptions of Rayleigh-Debye scattering and negligible secondary scattering. Thus, while the results of Fig. 3 motivate additional study of aggregate optical properties they should not be considered definitive.

Current work involves measuring the H/C ratios of soot, to indicate potential refractive index variations, and soot optical properties, to test the approximate aggregate optical theory.

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8. Ü.Ö. Köylü, and G.M. Faeth, "Emissions of Soot and Carbon Monoxide from Liquid Fueled Buoyant Turbulent Diffusion Flames," Proceedings of 24th Fall Technical Meeting, Eastern Section of the Combustion Institute, Pittsburgh, PA, submitted.
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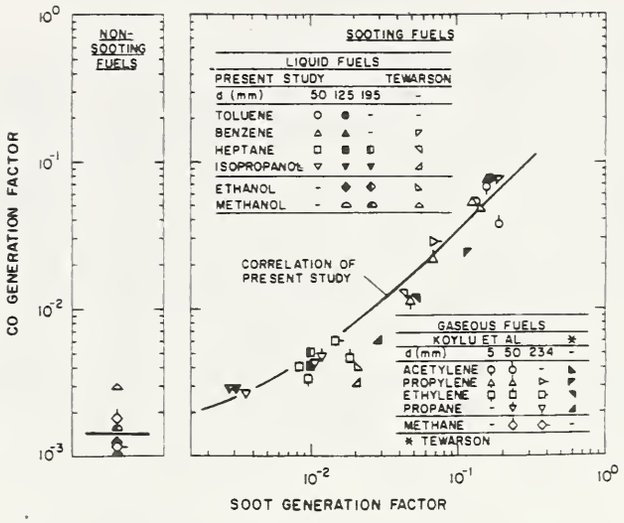


Fig. 1. Correlation between CO and soot generation factors.

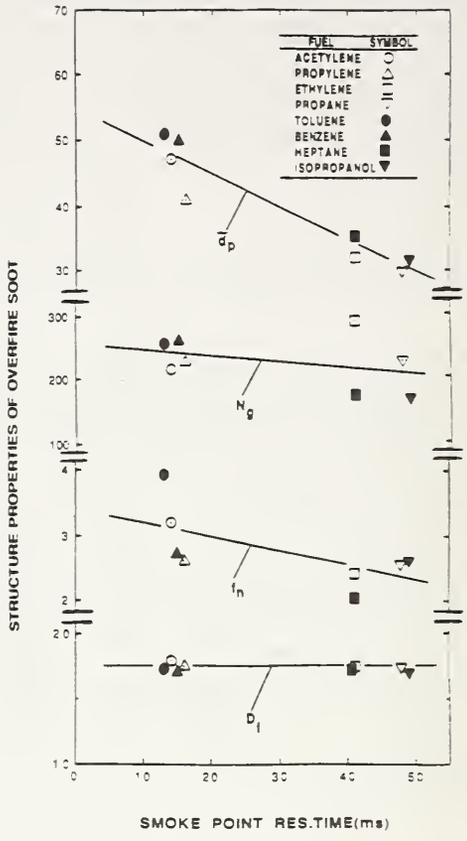


Fig. 2. Correlation between soot structure and sooting tendency.

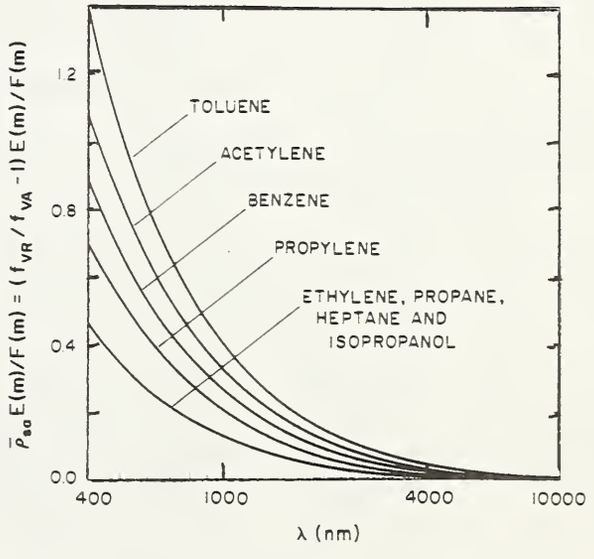
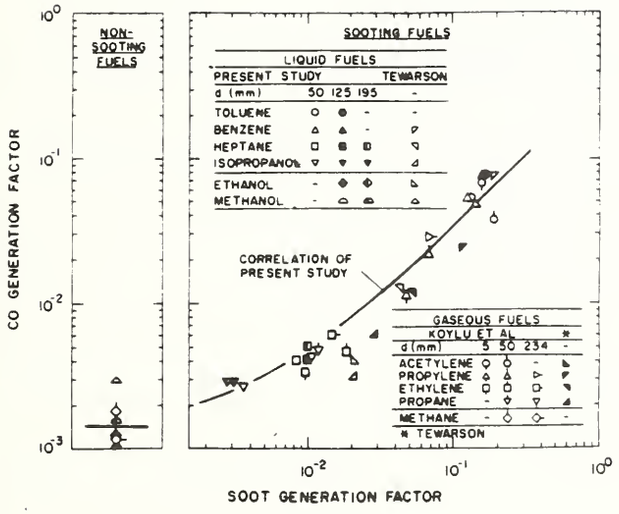


Fig.3. $\bar{\rho}_{sa}$ as a function of λ and fuel type.



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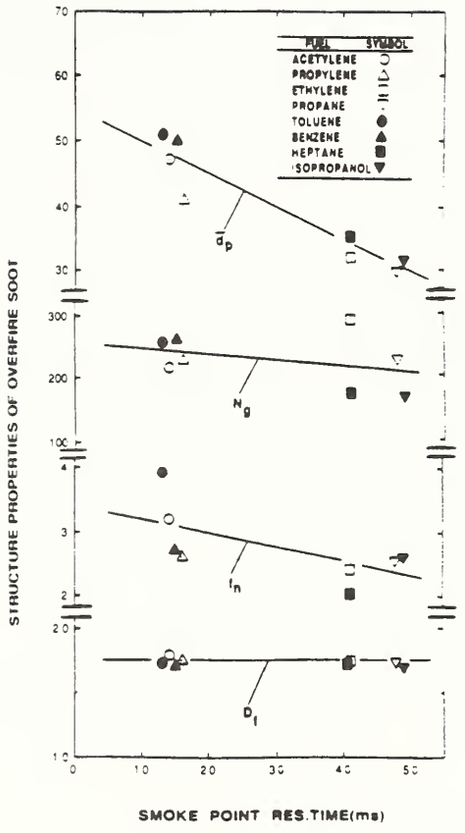

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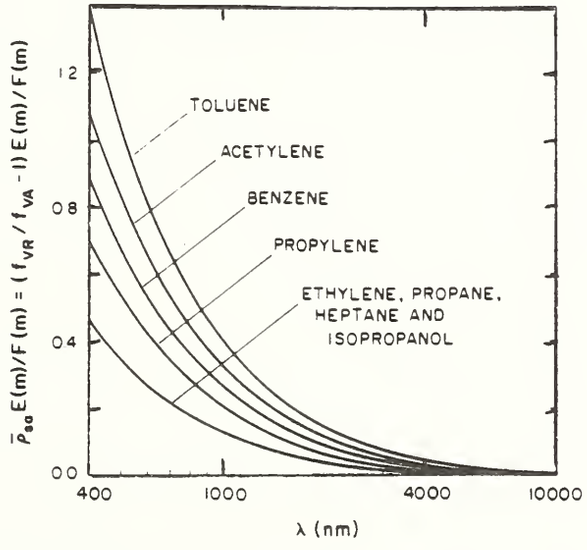

Fig.3. $\bar{\rho}_{sa}$ as a function of λ and fuel type.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution: The George Washington University

Grant Number: 60NANB9DO963

Grant Title: Simplifications of Diffusion Flame Chemistry: A Theoretical and Experimental Study of the Structure of Laminar Diffusion Flames

Principal Investigator: Professor J. Houston Miller
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Other Personnel: Mr. Bijon Ahvazi, Graduate Student
Ms. Elizabeth Abraham, Graduate Student

NIST Scientific Officer: Dr. Kermit C. Smyth

Technical Abstract:

Tunable Diode Laser Absorption Studies of Laminar Diffusion Flames

Introduction: Progress in modelling combustion systems requires a data base that can be used to validate not only the shapes and locations of profiles, but also absolute concentrations for flame species. Traditional sampling and analysis methods, such as quartz microprobe/mass spectrometry, are limited to flame regions that are relatively free of particulate matter, which clogs the small probe orifices required to achieve satisfactory spatial resolution. With some exceptions, many of the optical diagnostics methods employed so far are not quantitative, and may also suffer interferences from particulates and/or polynuclear aromatic hydrocarbons. Tunable diode lasers have been shown to be effective tools for both species and temperature measurements in combustion systems. In the past year, we have demonstrated their use for the determination of temperature and the concentration of carbon monoxide using both direct absorption and modulation techniques in laminar diffusion flames.

Temperature Measurements: It has been demonstrated that absorption across two spectrally adjacent carbon monoxide rotational lines which originate in different vibrational levels can be used to determine the flame temperature [1,2]. Figure 1 shows simultaneous fits of the CO P(4) ($1\leftarrow0$, 2127.68 cm^{-1}) and R(2) ($2\leftarrow1$, 2128.01 cm^{-1}) lines at 9 mm HAB and -3.8 mm from the burner centerline. For this calculation, it was assumed that both lines had the same room temperature collision halfwidth. Thermocouple measurements gave 1367 K for the temperature at this flame location [3](after a radiation correction had been applied), in excellent agreement with the temperature from the fit of this data: 1356 K.

Because of low absorption levels, measurements of carbon monoxide concentration and temperature at the lean edges of the flame (position greater than $\approx$ 6.5 mm from the burner

centerline) are unreliable with the direct absorption technique. It has been demonstrated that the sensitivity of tunable diode laser measurements could be increased by modulating the laser wavelength [4]. If the modulation frequency is less than the feature width then the technique is known as wavelength modulation or derivative spectroscopy. For derivative spectroscopy an oscillation is applied to the diode current as it is being scanned through an absorption feature. If the signal is sampled at twice the modulation frequency (known as *2f* detection), the processed signal will be the second derivative of the detector signal. Figure 2 compares the TDL measurement of the temperature profile 9 mm above the burner surface with the thermocouple measurements (solid lines). As the data in Figure 2 indicates, TDL absorption provides a reasonably accurate measurement of temperature in this flame

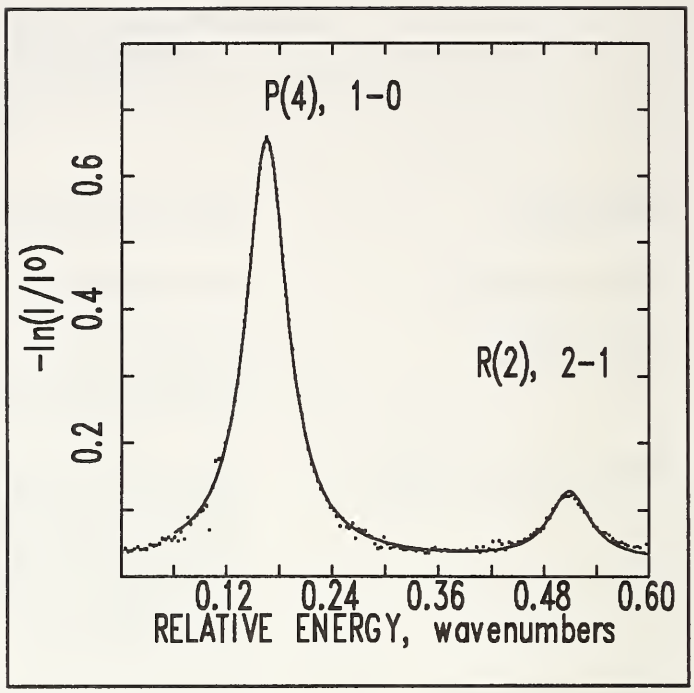

Figure 1

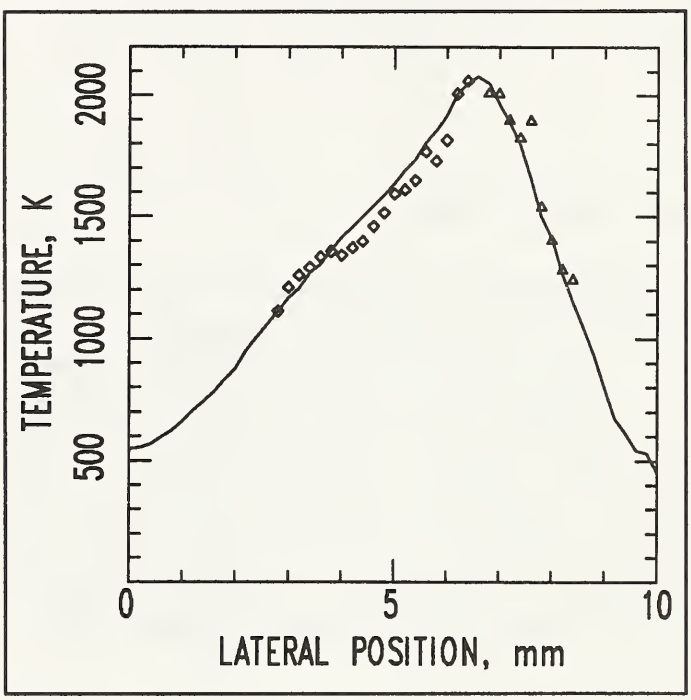

Figure 2

system: we conservatively estimate the direct absorption measurements (◊) to provide accuracy of ± 100 K and the centerline harmonic signal (△) to be good to ± 200 K. Moreover, the shape of the temperature profile is nearly identical for the two techniques. Improved accuracy might be possible by selecting CO line pairs which exhibited a greater dependence of line strength ratio on temperature [1,2].

Concentration Measurements: Figure 3 shows the concentration profile calculated from CO P(8) rotational line spectra (■) at a height of 9 mm above the burner surface. Data from -6.6 mm to 6.6 mm were from fits of the direct absorption signals. Concentrations outside of ± 6.6 mm were from wavelength modulation measurements. Also shown is a profile determined from quartz microprobe/mass spectrometer measurements (◊) and a relative profile of CO mole fraction determined from a laser induced fluorescence measurement (△) [5,6]. This figure shows good agreement between the three measurements of carbon monoxide concentration.

Modelling the Growth of Polynuclear Aromatic Hydrocarbons in Diffusion Flames

It has been noted for some years that the concentrations of many species in laminar hydrocarbon diffusion flames correlate with mixture fraction, or alternatively, local equivalence ratio.

Therefore, once the spatial profile for the mixture fraction is established, it is possible to approximate both the concentration and net chemical rate profiles for a great many flame species. However, some species exhibit concentration gradients along contours of constant mixture fraction in a flame. The results of our past work shows that most of the species along the chemical pathway leading to soot particle formation in diffusion flames, including all of the Polynuclear Aromatic Hydrocarbons, exhibit this type of behavior. For these species, it is necessary to consider not only the chemistry of the growth environment, which may be adequately described by the mixture fraction, but also the residence time within the growth region. During the last year we developed a model which describes the physical and chemical processes that affect PAH and soot concentrations along a stream line in a laminar methane/air diffusion flame. The development is similar in spirit to that presented in a recent paper by Kennedy et al. [7]. In both models, soot processes are divided into three broad categories: inception, chemical growth, physical growth (agglomeration), and oxidation. Both assume that the rate of the soot processes depends on local temperature and the concentrations of major species, and these are fully determined by mixture fraction. However, rates of these processes in the Ref. 7 were derived from either empirical data or was a variable parameter in the model. In our model, we attempt to rationalize the choice of rates based on a knowledge of the fundamental chemical processes which are occurring in the flame combined with detailed measurements of species concentrations.

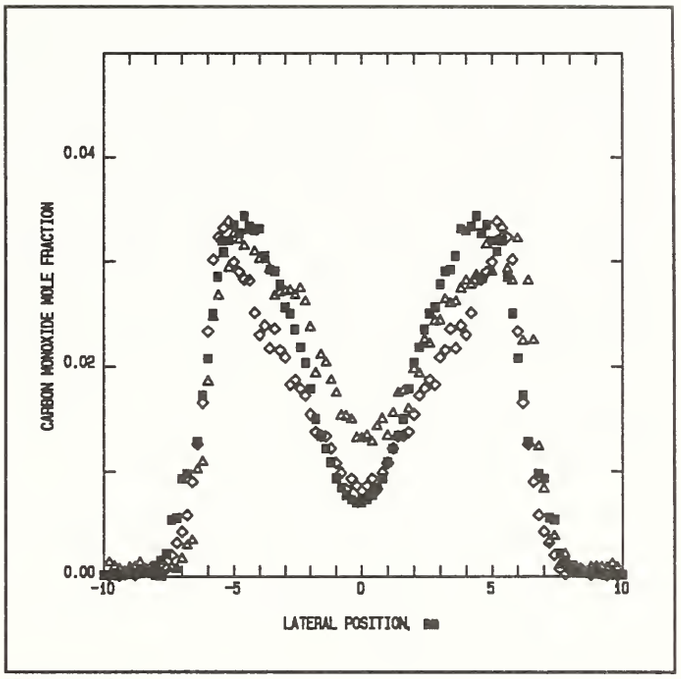

Figure 3

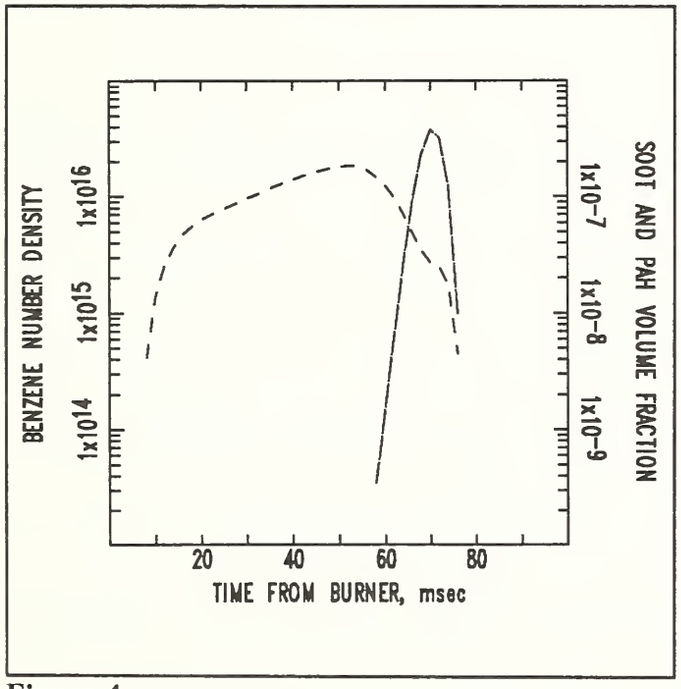

Figure 4

The concentrations of polynuclear aromatic hydrocarbons have been calculated along a series of streamlines in a laminar axially symmetric methane/air diffusion flame and are shown in Figure 4. The model was first run using an expression for the effective rate constant for chemical growth derived form local temperature, and the concentrations of C_2H_2, H_2, and H· correlated against mixture fraction from the Wolfhard-Parker flame data. It should be noted that H-atom plays a critical role in this chemistry: abstraction of ring hydrogens from the PAH is responsible for "activating" the surface for further growth. Unfortunately, in the flame region that growth is likely to occur, there are no reliable measurements of H-atom concentration [8]. In these flame regions we have calculated [H·] assuming total local equilibrium. There has been much written about the importance of super-equilibrium concentrations of radicals in combustion processes in

general [9] and aromatic growth in particular [10]. Although it is well known that super-equilibrium exists near the high temperature reaction zone of hydrocarbon diffusion flames, calculations also suggest that super-equilibrium extends well into the fuel rich flame regions where growth may occur [9]. Therefore, assumption of total equilibrium may grossly underpredict the concentration of hydrogen atoms and, consequently, the rate of ring growth. Our model calculations bear this out: unless an enhancement factor for chemical growth was included, no appreciable build-up of PAH occurs. To reach a volume fraction of soot approaching that which has been observed experimentally [11], this factor must be on the order of 500, which implies hydrogen atom concentrations in the growth region on the order of a few hundred parts per million. With current measurement strategies for hydrogen atom, this is a value near the detection limit in fuel rich regions of a diffusion flame [6].

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1) "The Kinetics of Polynuclear Aromatic Hydrocarbon Agglomeration in Flames", J.H. Miller, **The Twenty-third International Symposium on Combustion**, (The Combustion Institute, Pittsburgh, 1990) pp. 91-98.
2) "Comparisons of Methane/Air Diffusion Flame Structure Data with Predictions of Full and Reduced Chemical Mechanisms."
J. Houston Miller and K.C. Smyth, **Chemical and Physical Processes in Combustion**, Paper 37, (1990).
3) "Modelling the Growth of Polynuclear Aromatic Hydrocarbons in Diffusion Flames."
J.H. Miller, D.R. Honnery, and J.H. Kent, **Symposium on Combustion Chemistry**, American Chemical Society Fuel Division Preprint, Paper 18 (1991).
4) "An Infrared Fault Detection Method for Hazardous Waste Incineration."
J.T. McKinnon, E. Abraham, and J.H. Miller, **Combust. Sci. Technol.**, submitted for publication.
5) "Tunable Diode Laser Measurement of Carbon Monoxide Concentration in a Laminar Methane/Air Diffusion Flame."
J.H. Miller, S Elreedy, B. Ahvazi, F. Woldu, and P. Hassazadeh, **Appl. Optics**, submitted for publication.

1.2 Soot Formation

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - 1991

SOOT FORMATION AND EVOLUTION

Professional Staff

Kermit C. Smyth, Project Leader
George W. Mulholland, Project Leader
Nelson P. Bryner, Chemical Engineer
J. Houston Miller, Visiting Scientist

Project Objectives

Develop scientifically sound principles, metrology, and data which contribute to a predictive model for the formation and evolution of smoke components in flames based upon the best available information for use in understanding general fire phenomena.

Scope

This work embraces broad areas underpinning BFRL Fire Research Program programs with focussed study of hot gas chemistry and physics. Efforts are directed toward improved understanding of the chemical and physical processes which underlie macroscopic fire phenomena and include development of new techniques and methods for studying these processes.

Technical Accomplishments

During hydrocarbon combustion the exothermic chemical reactions which lead to the formation of water and carbon dioxide consume most of the fuel. However, in many cases a significant fraction of the fuel is converted into species which participate in chemical growth reactions. These processes lead to dramatic consequences in numerous combustion environments. For example, the formation of intermediate hydrocarbons, such as polycyclic aromatic hydrocarbons (PAH), occurs under fuel-rich conditions and poses a potential long term health hazard since many PAH are carcinogenic. In addition, such compounds are also involved in further growth reactions to form soot particles. Radiation from soot dominates energy transfer from large fires, and thus soot formation plays a key role for combustion efficiency in furnaces and for flame spread. In turn, particle formation and radiative energy transfer control the amount of smoke produced, which is important in fire detection and pollutant emission. In contrast to the oxidation of simple hydrocarbons, which is well understood, the detailed mechanisms for producing large hydrocarbons during combustion have not been established. The elucidation of chemical growth mechanisms continues to be one of the most challenging research problems in combustion science today.

While the chemical growth reactions play a key role in regard to the total amount of smoke produced, the actual structure of the smoke leaving the flame region is determined by a physical agglomeration process of particles sticking and forming a cluster. The agglomerate structure consists of a number of primary particles with diameters of about 30 nm connected in a rather open structure.

The light extinction coefficient and light scattering coefficient, both of which affect the visibility through smoke, are not well characterized for agglomerate structures. The aerodynamic properties, which control smoke deposition in the respiratory tract, are also poorly characterized. Understanding the relationship between the geometric structure of an agglomerate and its properties is a key research topic in both aerosol research and condensed matter physics.

1. Soot Formation

This project is part of a long-term study of the fundamental chemistry of soot formation. Detailed flame structure measurements (species concentrations, temperature, and velocity) have been made in a laminar methane/air diffusion flame using a variety of laser-based optical techniques as well as mass spectrometric sampling. Our recent emphasis has been to make accurate quantitative and relative profile measurements of the radical species.

We have undertaken a detailed comparison of our experimental species and temperature data with the flame structure calculations of Mitch Smooke at Yale. To this point few studies have addressed the question of how well flame structure calculations reproduce experimental results. Profile concentrations of OH•, H atom, O atom, CH•, and the methyl radical in a laminar CH_4/air flame have been reported. Of these, OH•, H atom, and CH_3• can be placed on a quantitative basis. Combined with mass spectrometric data on all of the major species in this flame, these radical concentrations can be analyzed in terms of the local mixture fraction. Comparisons have been made with Smooke's co-flow flame structure computations, wherein the local scalar dissipation rates in the region of the stoichiometric mixture fraction are matched as closely as possible. In general, the agreement is excellent, especially for the major radicals OH•, H atom, and O atom.

Recent measurements on OH• concentrations in the soot oxidation region of laminar CH_4/air and C_2H_4/air diffusion flames have also been carried out with Bob Santoro and his students. In the oxidation region there exists a competition for OH• between CO and soot particles, since OH• is a key oxidizer for each. Furthermore, the oxidation of soot itself leads to enhanced levels of CO. Previous work has shown that the emission of CO from diffusion flames is closely related to the observed soot concentrations within the flame, which in turn control smoke emission levels. Our objective is to unravel this competition for OH•; there are no available measurements of OH• in the presence of soot.

The flame structure calculations provide an excellent prediction of the OH• concentrations over the entire profile in the absence of radiation losses due to soot particles. However, when radiation losses are included, predictions of the temperature field and the degree of radical superequilibrium are difficult to make. The present work is intended to specifically establish how the OH• concentration varies as the soot concentration is changed. To do this, quantitative measurements of the soot, OH•, and CO concentrations as well as the surface area of the soot particles (or the primary particle size) and the temperature field in the oxidation region are needed. In addition, data on O_2 concentrations will enable us to address the question of whether OH• or O_2 is more important for the oxidation of soot particles. These data are essential input for an integrated soot formation model; the oxidation step for all of the soot models proposed thus far rests upon calculated or assumed quantities.

2. Smoke Agglomerates

A combined experimental and theoretical effort is focussed on the characterization of the optical properties of smoke agglomerates. The theoretical effort has consisted of generating simulated smoke

agglomerates of various sizes and then computing the light scattered by the agglomerates using Rayleigh-Debye scattering theory. The most noteworthy result of this analysis is the prospect of inferring information about the concentration and size of the soot from the scattering measurements. It is shown that from the scattering measurements one can infer the overall size of the agglomerate, the size of the primary units in the agglomerate, the number of primary units in the agglomerate, and the number concentration of agglomerates.

To study the optical properties of smoke, a combined transmission cell-reciprocal nephelometer has been developed. This device allows the simultaneous measurement of the extinction coefficient and the total scattering coefficient of smoke. These are the key quantities needed for studying radiation transport through a smoke cloud. From the difference of these two quantities, the absorption coefficient can be determined. During the past year a radiometric model has been developed for the transmission cell reciprocal nephelometer (TCRN). The model involves the computation of the light scattered from an infinitesimal element of the laser beam within the TCRN to an infinitesimal element of the cosine sensor. Integrating over the surface of the senor and along the laser beam yields the total flux of light reaching the cosine sensor. Calculations were carried out for smoke agglomerates by using the theory of fractal optics and for spheres by using Mie theory. The cluster size was varied from 10 spheres to 10^8 spheres for the fractal calculation and the sphere size was varied from 0.02 μm to 8 μm for the Mie scattering. Key issues in the analysis include the effect of the finite size of the detector, the finite length of the TCRN on the predicted total scattering, and the distance of the laser beam to the detector.

Recent experimental work has focussed on the design and testing of two solid cosine sensors, which were fabricated from opaque and translucent plastics. These new sensors allow the TCRN to operate at high and low pressures, and replace a flexible Teflon membrane sensor which deformed when it experienced a significant pressure differential. In addition, the 2.5 and 5.0 cm diameter sensors permit data to be collected as a function of size for comparison with model predictions. After laboratory testing, a solid sensor was used in the portable TCRN which was installed on NCAR's Electra aircraft to sample smoke from Kuwait oil fires. The ability of the solid sensor to withstand pressure fluctuations was critical for the operation of the TCRN because the aircraft sampled smoke at different altitudes.

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"Signal Detection Efficiency in Multiphoton Ionization Flame Measurements," K. C. Smyth and P. J. H. Tjossem, Applied Optics 29, (1990).

"Relative H-Atom and O-Atom Concentration Measurements in a Laminar, Methane/Air Diffusion Flame," K. C. Smyth and P. J. H. Tjossem, Twenty-Third Symposium (International) on Combustion, (1991).

"The Kinetics of Polynuclear Aromatic Hydrocarbon Agglomeration in Flames," J. H. Miller, Twenty-Third Symposium (International) on Combustion, (1991).

"Laser-Induced Fluorescence of CH· in a Laminar CH_4/Air Diffusion Flame: Implications for Diagnostic Measurements and Analysis of Chemical Rates," T. S. Norton and K. C. Smyth, Combustion Science and Technology Vol.76, (1991).

"Polycyclic Aromatic Hydrocarbon Emissions from the Combustion of Crude Oil on Water," B.A. Benner, N.P. Bryner, S.A. Wise, and G.W. Mulholland, Environmental Science and Technology 24, (1990).

"Smoke Emission and Burning Rates for Urban Structures," N.P. Bryner and G.W. Mulholland, Atmospheric Environment 25A, (1991).

"Ultrafine Combustion Aerosol Generator," T. Cleary, R. Fletcher, L. Ives, G.W. Mulholland, and J. Gentry, submitted to Aerosol Science and Technology.

Related Grants

"Soot Morphology in Buoyancy Dominated Flames," Richard A. Dobbins, Brown University.

"Modelling of Soot Formation in Diffusion Flames," Ian Kennedy, University of California at Davis.

"Simplifications of Diffusion Flame Chemistry: A Theoretical and Experimental Study of the Structure of Laminar Diffusion Flames," J. Houston Miller, George Washington University.

"Fundamental Mechanisms for CO and Soot Formation in Diffusion Flames," Robert J. Santoro, Pennsylvania State University.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 91

Institution: The Pennsylvania State University

Grant No.: 60NANB01035

Grant Title: Fundamental Mechanisms of CO and Soot Formation in Diffusion Flames

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Other Professional Personnel: T. F. Richardson, Doctoral Student
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Technical Abstract:

Introduction. Carbon monoxide and soot represent the most serious combustion products formed in fires with respect to loss of life and injury. Consequently, an understanding of processes which control their formation and destruction is critical to fire modeling and impact mitigation. The high concentrations of CO and soot that characterize typical fire situations are recognized to be interrelated. The fundamental nature of this interaction is being investigated in this study. Two possible mechanisms that could affect the concentration of CO in the presence of soot, namely radiative quenching and competition for oxidizer species, are being examined. In the past, equilibrium estimates of OH concentration have been used to determine that radiative quenching can account for the higher CO observed in the fuel lean regions of diffusion flames [1]. The soot oxidation rates, based on surface area evaluated from optical measurements alone, allowed the inference that competition between CO and soot for OH in both fuel lean and fuel rich regions of the flame could also contribute to the higher CO emissions [1]. However, uncertainties in the soot surface area and the OH reaction efficiency with soot precluded a quantitative evaluation of the relative importance of these two mechanisms. Therefore recent efforts have focussed on measuring the OH concentration and improving estimates of soot surface area using Transmission Electron Microscope (TEM) measurements of primary particle size.

OH Measurements. Laser-induced fluorescence (LIF) was utilized to measure OH concentrations in a series of methane and ethene laminar diffusion flames burning in air. The burner, which is coannular in geometry, has been extensively described [2]. It consists of a 1.11 cm fuel tube surrounded by a 10.18 cm air annulus. Both methane and ethene fuels were studied at volumetric flow rates corresponding to 7.7 cm^3/s for methane and 3.85, 4.6 and 4.9 cm^3/s for ethene. The air flow rate for the methane flame and the 3.85 cm^3/s ethene flame was 1062 cm^3/s and, for the higher ethene flow rate flames was 1298 cm^3/s. For the ethene flame having the lowest fuel flow rate, no soot is observed to survive the flame tip, while for the largest fuel flow rate case soot is clearly observed to issue from the flame. For the 4.6 cm^3/s flow rate, the flame is quite close to the smoke point condition [3]. In addition to the coannular flame measurements, profile measurements were made in a Wolfhard-Parker flame using methane as the fuel. These studies were carried out to provide a comparative basis from which to determine the absolute OH concentration in the coannular flames.

The LIF measurements were made using a Nd:YAG pumped dye laser whose output was frequency doubled to produce light at 278.83 nm and 283.55 nm. These wavelengths excite the $S_{21}(8)$ and the $Q_1(8)$ lines of the $A^2\Sigma^+ \leftarrow X^2\Pi_i$ (1,0) band of OH respectively and were selected to minimize the variation of the rotational population level with temperature. Fluorescence was measured at 90° using longpass glass

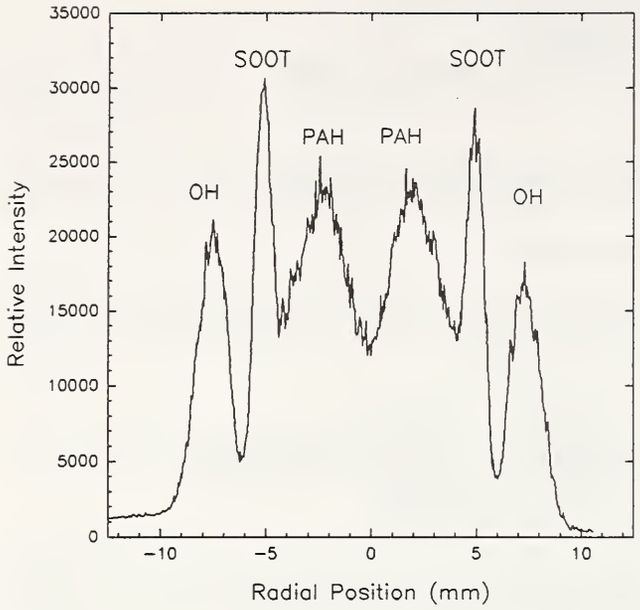

Figure 1. Laser-Induced Fluorescence in the axisymmetric ethene flame (Fuel flow rate = 3.85 cm^3/s, H = 7 mm).

filters which minimized elastically scattered light while transmitting the (0,0) band emission of OH at 308 nm.

In order to calibrate the peak OH concentration in the coannular burner the following steps were taken. First, point profile measurements were made in a methane-air flame stabilized on the rectangular slot (Wolfhard-Parker) burner, where previous absorption measurements have established the peak OH concentration [4]. Next, LIF signal levels in the methane-air flame on the rectangular slot burner were compared with those from the methane-air flame on the axisymmetric burner. Point profile measurements were also made in the ethene flame with the lowest flow rate.

For the fluorescence measurements in the coannular burner, light detection was accomplished using a cooled CCD detector with camera control and data storage with a 386 personal computer. Both 1D line and 2D planar images of the resulting fluorescence were recorded. The 1D line images were obtained by exciting the $S_{21}(8)$ OH line, while the 2D planar images were obtained by exciting the stronger $Q_1(8)$ OH line. The results presented here are raw signals and need to be corrected for the variations in laser pulse energy and the local quenching rate.

An example of a typical fluorescence profile is shown in Figure 1. Three distinct contributions are observed from OH, soot and polynuclear aromatic hydrocarbon (PAH) species [5]. When the laser was tuned off resonance with respect to the OH rotational line, the two peaks furthest from the burner centerline disappeared, while the features attributed to soot scattering and PAH fluorescence remained.

Figure 2 shows a series of OH fluorescence intensity profiles for several axial positions in the methane flame. The soot and PAH signals have been eliminated by subtracting the off resonance profile from the on resonance profile at each axial location. These results show a clear trend in the concentration profiles. The relative intensity decreases in magnitude and increases in spatial extent with height in the flame. The results for the ethene flame having a fuel flow rate of 3.85 cm^3/s show similar trends. It should be noted that the ethene flame has nearly an order of magnitude more soot than the methane flame.

The OH concentrations are difficult to determine in the soot region at higher heights in the ethene flames with higher fuel flow rates (and consequently higher soot concentrations). This is due to problems associated with the subtraction of two large soot signals relative to a much smaller OH signal. The 2D planar data were obtained using a stronger $Q_1(8)$ line and thus showed much larger OH signals relative to the soot scattering signals. Figure 3 presents the profiles obtained with the laser tuned both on and off resonance for the ethene sooting flame at a height of 100 mm. OH is present throughout the region where soot breaks out of the flame. Figure 4 shows the net OH signal obtained by subtracting the off resonance profile from the on resonance profile. Thus these results demonstrate the capability to measure OH concentration variations in the region of the diffusion flame tip where soot and CO oxidative steps compete for OH.

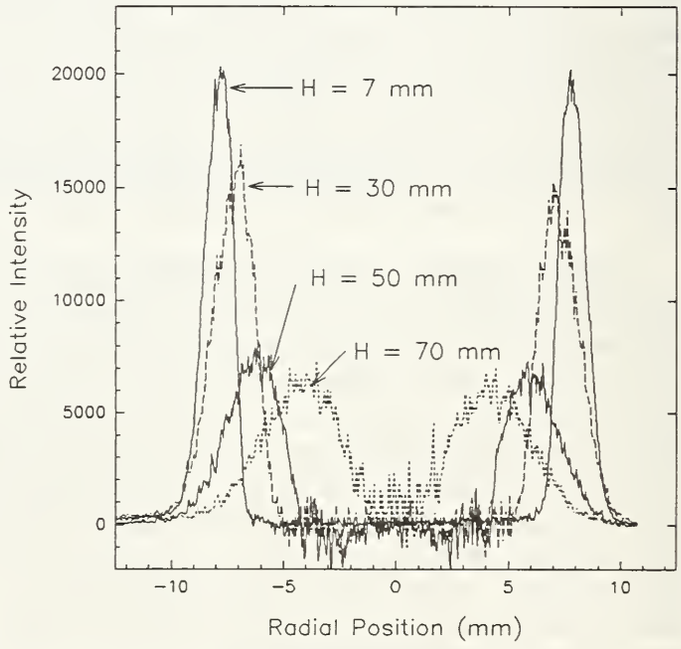

Figure 2. OH intensity profiles in the methane flame. Visible flame height = 79 mm.

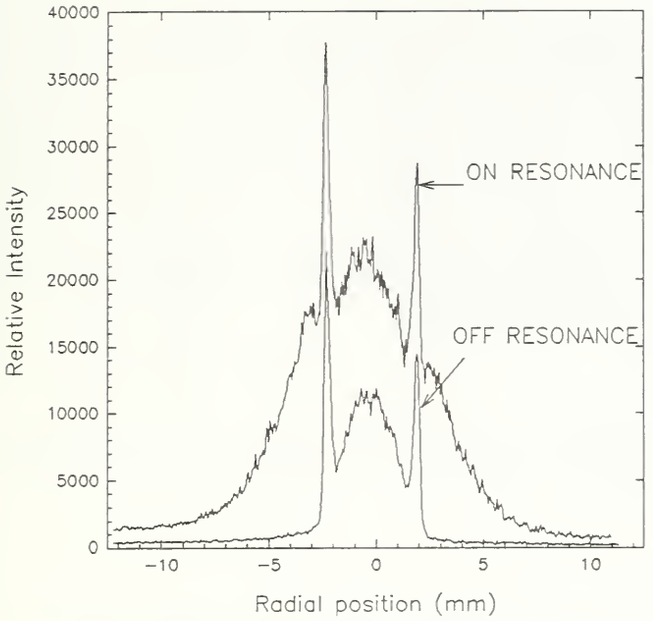

Figure 3. On and off resonance profiles for the sooting ethene flame (Fuel flow rate = 4.9 cm^3/s, H = 100 mm).

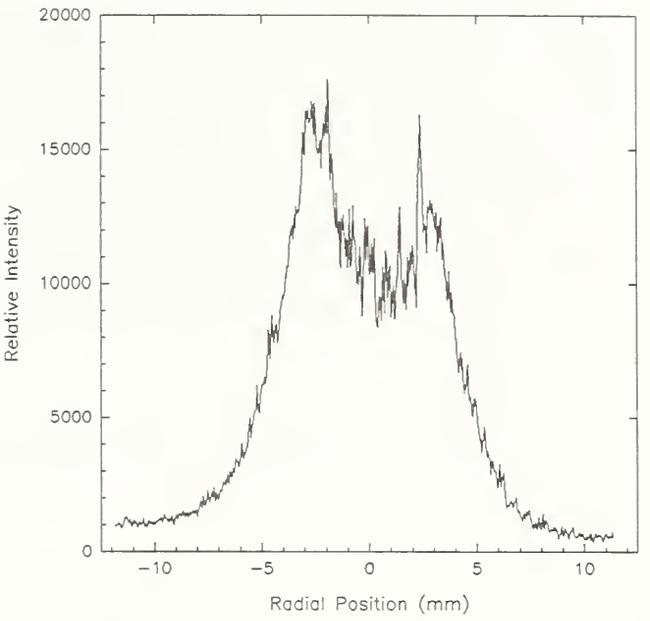

Figure 4. OH profile in the soot emitting ethene flame at H = 100mm.

TEM Measurements. The optical measurements of soot assume spherical particles and do not accommodate their aggregate nature. Consequently soot oxidation rates based on these measurements alone can be significantly in error. Thermophoretic sampling of soot aggregates on TEM grids yields primary particle size information, d_p, which, in combination with optical measurement of volume fraction, f_v, can give more accurate soot oxidation rates.

Thermophoretic sampling takes advantage of soot particle transport to a cold surface in the presence of a temperature gradient [6]. The thermophoretic probe consists of a carbon coated 200 mesh copper grid held in place between two strips of sheet metal, machined to expose the grid to the flame. The probe is rapidly located in the flame environment, exposing the grid to the soot field for 50 msec. This short exposure time provides a cold surface to quench the heterogeneous reactions on the captured particles. The TEM negatives at a magnification of 60K were imaged with a CID camera and the image analysis software was used to measure the primary particle sizes.

Figure 5 shows the temporal variation of primary particle size, d_p, along the centerline of a flame burning a mixture of methane and 1-butene. This flame, like the highest ethene flow flame, emits soot. The primary particle diameters shown in Figure 5 are arithmetic averages of 100 measurements or more at each temporal location. Since the measurements were made along a streamline, the number of primary particles, N_p, can be expected to be constant [7]. This intuitive observation can be exercised as a useful consistency check of the d_p and f_v measurements. This consistency check is currently in progress and soot oxidation rates based on these measurements will be forthcoming.

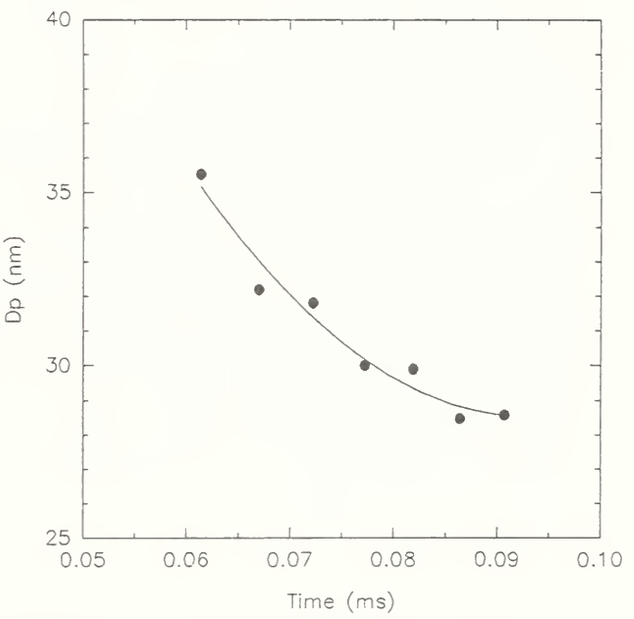

Figure 5. Temporal profile of the primary particle size, d_p, in the methane/1-butene flame.

Summary. One of the major objectives of the current study is to provide a quantitative basis from which to assess the competition between CO and

soot for OH species. In particular, it is desired to estimate the degree to which temperature reductions due to increased radiation from soot as compared to soot oxidation by OH are responsible for the higher levels of CO observed as the soot concentration increases [1]. Consequently, the OH concentration variation near the tip of the flame has been examined for non-soot emitting, near soot emitting and soot emitting conditions. Once the relative intensity profiles are converted to absolute OH concentrations and the TEM observations are checked for consistency, the previously measured soot volume fraction, CO, velocity and temperature fields can be used to evaluate the relative contributions of the temperature and reactive competitive mechanisms to the CO emissions observed for flames with increased soot loading. Based on these results, the fundamental mechanisms important in the formation and destruction of CO with respect to soot in fires can be incorporated into current fire models.

Acknowledgement

The hydroxyl radical measurements were obtained in collaboration with Dr. Kermit C. Smyth of the Building and Fire Research Laboratory and his contributions are gratefully acknowledged.

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5. Puri, R., and Santoro, R.J., "Sonic Probe Sampling in Particle Laden Flows"' Eastern Section: The Combustion Institute, fall Technical Meeting, Orlando, FL, December, 1990.
6. Santoro, R.J., Puri, R., Richardson, T.F., and Dobbins, R.A., "Interactive Use of Electron Microscopy and Light Scattering/Extinction Tests in Particle Formation Diagnostics. II. Light Scattering and Extinction Tests, Tenth Annual Meeting, American Association for Aerosol Research, Traverse City, October 7-11, 1991.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution: University of California Davis
Grant No. : 60NANBOD1055
Grant Title: Modelling of Soot Formation in Diffusion Flames
Principal Investigator: Dr. Ian M. Kennedy
Other Professional
Personnel: Dr. Rafael Villasenor, Post-doctoral Researcher
NIST Scientific Officer: Dr. Kermit Smyth
Technical Abstract

INTRODUCTION

The project seeks to develop a useful model for soot formation and oxidation in laminar diffusion flames with ultimate application to modelling smoke formation from turbulent diffusion flames that are typical of fires. A semi-empirical approach has been used; experimental results for specific surface growth rates on soot particles are an input to the model. Conservation equations for the flow field and the soot volume fraction are solved. The results of this modelling exercize are compared witht experimental results from an ethylene air diffusion flame. A major test of the modelling is the prediction of flame sooting heights. The model offers new insights into the relationship between soot concentrations, OH concentrations and CO emissions.

OVERALL APPROACH

The model solves the boundary layer form of the flow equations which include the continuity equation, momentum equation, mixture fraction equation, enthaply equation, and the transport equation for the soot volume fraction. In the new formulation of the model the radiation heat loss, which is critical in predicting the flame temperatures, is explicitly considered in the energy equation. The thermo-chemical properties are obtained from an equilibrium calculation as a function of mixture fraction and enthalpy at one atmosphere.

GOVERNING RATES

The rate of particle formation, W_n, is modeled as a Gaussian distribution in mixture space centered at a mixture fraction of $f^*=0.1$, with standard deviation $\sigma=0.08$. The maximum particle production rate is determined by assuming an initial particle diameter of 1nm and a peak formation rate of 10^{20} $m^{-3}s^{-1}$.

The soot surface growth rates, W_g, are determined with an empirical correlation between mixture fraction and the specific surface growth rate. The values for the specific surface growth rates, s, as a function of mixture fraction, f, are obtained from measurements of a laminar, ethylene stagnation point diffusion flame. The temperature dependence is assumed to be given by an Arrhenius equation. The modeled activation energy value is $E_a=20$ Kcal/mol and the local gas temperature is compared to the adiabatic equilibrium temperature to give the local specific surface growth rate. The growth rate given in terms of the above variables has the following form

$$W_g = \pi^{1/3} 6^{2/3} \phi^{2/3} N^{1/3} S(f,T) \qquad (1)$$

where

$$S(f,T) = \frac{3}{2} s(f) \exp\left[-E_a\left(\frac{1}{T} - \frac{1}{T_{eq}}\right)\right] \quad (2)$$

The computation of the surface growth rate as given by Eq. (1) requires, in principal, an additional transport equation for the particle number density. However, it is possible to neglect the variations in number densities with minor effect on the results and to adopt a suitable average number density, N_{avg}. In our study the previously chosen value of 10^{16} m^{-3} is used in all calculations.

Particle oxidation has been included through the action of both OH radicals and O_2. The rate of combustion of soot due to molecular oxygen is determined form the Nagle and Strickland-Constable formula. The rate of OH attack is evaluated from kinetic theory collision rate with a reaction efficiency of 0.2. The rate of conversion

$$W_{OH} = 10.14 \alpha \phi^{2/3} N^{1/3} X_{OH} T^{-1/2} \quad (3)$$

is expressed in m^3_{soot} m^{-3} s^{-1}. The overall rate of oxidation is the sum of the terms given for OH and O_2 attack.

RESULTS

Comparisons have been made with the measurements of Santoro et al and with Kent and Wagner. Both groups used co-flow laminar ethylene flames. Santoro studied flames at four different flow rates; these flames will be referred to hereafter as Flames 1, 2 3 and 4. A useful basis for comparison of the soot in different flames is the so-called integrated soot volume fraction that is defined below:

$$F_v(\eta) = 2\pi \int_0^R \phi(r,\eta) r dr \quad (4)$$

where f is the local soot volume fraction and η is the non-dimensional axial coordinate. The quantity η is given as

$$\eta = [xD / Q] ln(1 + 1/P) \quad (5)$$

where x is the axial distance (cm), D is the diffusion coefficient which is taken to be 0.156 $cm^2 s^{-1}$, Q is the volumetric flow rate ($cm^3 s^{-1}$) of fuel and P is the stoichiometric ratio of the volume of air to volume of fuel (P=14.28 for ethylene-air). The definition of η is chosen to provide a scaling approach for F_V in terms of the maximum soot volume fraction and general shape of the curves for the various flames studied.

Figures 1 through 4 show the integrated soot volume fraction. The location of the peaks in F_V are almost centered around η=0.1 which indicates that the flames exhibit the expected similarity behavior. Also note that as the fuel flow rate is increased the flames have greater nondimensional length. Flames 1 and 2 are nonsmoking flames. The smoke point flow rate is clearly indicated by the profile of flame 3. Here the integrated soot volume fraction does not decay abruptly in the oxidation zone; it persists into the air side of the flame. The agreement between predictions and measurements is excellent except for flame 1 where the model predicts higher oxidation rates. In Figure 4 a horizontal region appears just after soot burnout ceases, indicating that this flame emits smoke. The numerical results and the experimental data for flame 4 compare well in both the formation and burnout regions but a discrepancy is observed at the tip of the flame where the model

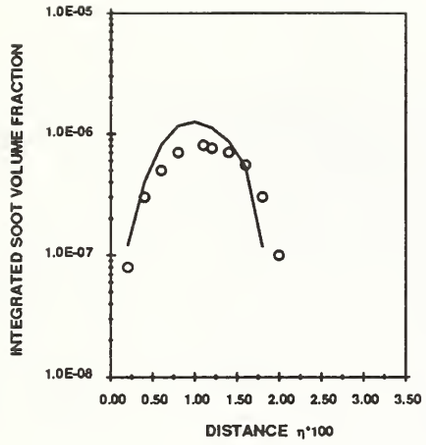

Fig. 1 Integrated soot volume fractions in Flame 1 of Santoro et al

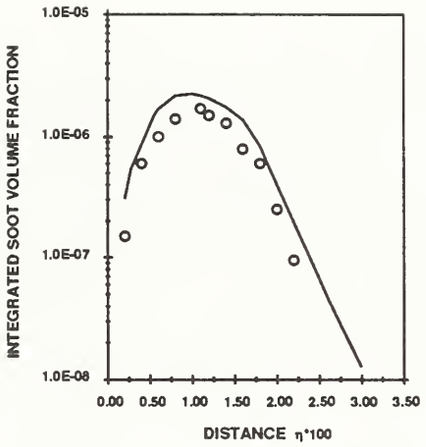

Fig. 2 Integrated soot volume fractions in Flame 2 of Santoro et al

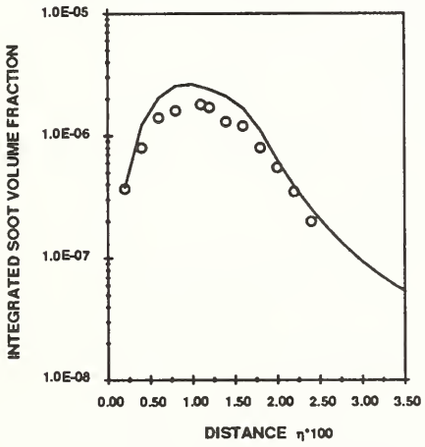

Fig. 3 Integrated soot volume fractions in Flame 3 of Santoro et al

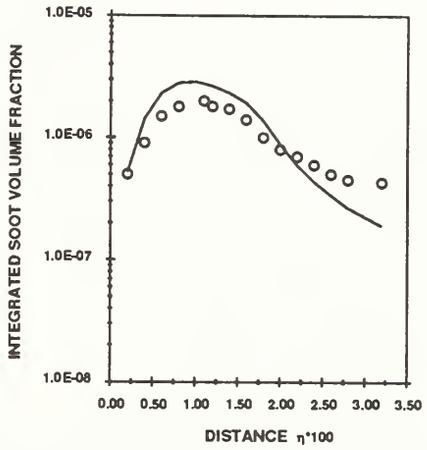

Fig. 4 Integrated soot volume fractions in Flame 4 of Santoro et al

underpredicts the amount of soot that is emitted. Although not shown here, the results for the Kent and Wagner round ethylene flame are equally as encouraging. The transition to a sooting flame is predicted very well.

The oxidation rates due to the OH and O_2 species are shown in Fig. 5 for flame 4 at axial locations x=40, 51, and 70 mm. These curves give clear evidence of the effect that the oxidants have on the soot particles at various positions in the flame. Just above the

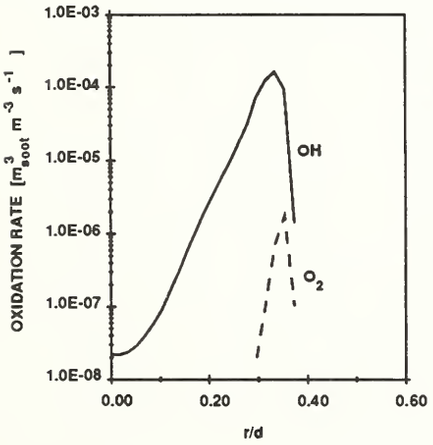

Fig. 5a Oxidation rates in flame 4 at x/D=40mm

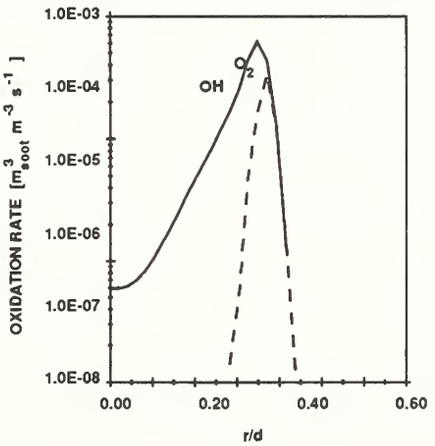

Fig. 5b Oxidation rates in flame 4 at x/D=51mm

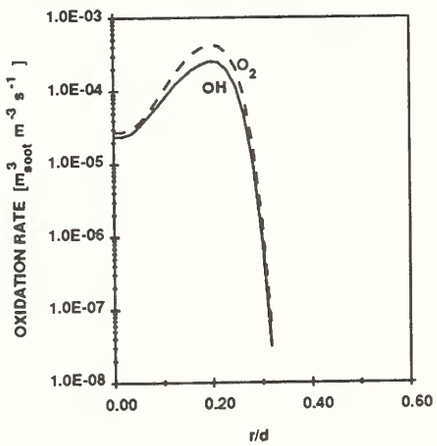

Fig. 5c Oxidation rates in flame 4 at x/D=70mm

burner (Fig. 5a), soot particles are oxidized mainly via the OH radicals. The contribution to oxidation by O_2 is negligible because of the low O_2 concentration. By contrast, at the flame tip (Fig. 5c), the contribution by O_2 to the burnout process as predicted by the Nagle Strickland-Constable formula is more important than the OH contribution.

In order to shed light on the question of OH loss on soot particles, the calculations of an ethylene counterflow diffusion flame with detailed chemistry have been analyzed. A sink term was included in the energy equation to model the effects of radiation; the flame temperature was about 1710 K which is comparable to the temperatures found near the major soot burnout zone. With the detailed results for all mole fractions, temperatures and velocity a convection-diffusion-reaction balance is performed to extract the net formation rate of OH as a function of mixture fraction. The results of this exercise are shown in Fig. 6.

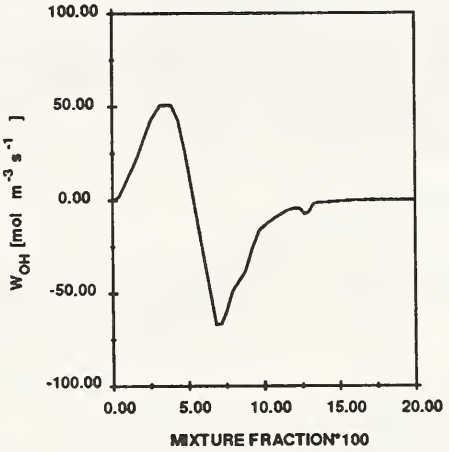

Fig. 6 Net formation rate of OH in counterflow ethylene flame

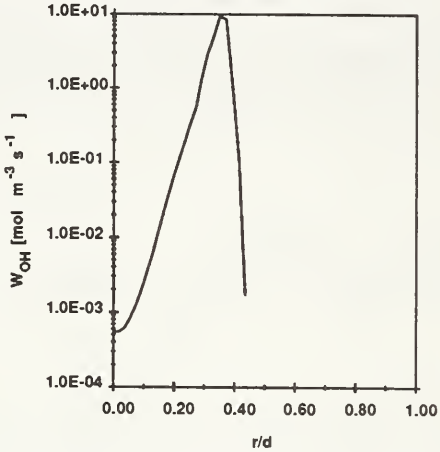

Fig. 7 OH loss rate on soot at x/D=50 mm in flame 4 of Santoro et al

The net OH formation rates that are shown in Fig. 6 may be compared with the inferred OH loss rates on soot particles that have been obtained with the present model of the co-flow ethylene flame of Santoro et al. The results of this comparison are shown in Fig. 7. It is apparent that there is a factor of five difference. In view of the uncertainties and possible underestimation of OH concentrations, for example, the comparison suggests that soot may present a significant route for the loss of OH from a diffusion flame near the tip with a concomitant effect on CO oxidation and with the potential for local extinction of the flame itself.

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BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 91

Institution: Brown University

Grant No.: 60NANB1D1110

Grant Title: Soot Morphology in Buoyancy Dominated Flames

Principal Investigator: Prof. R. A. Dobbins
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Professional Personnel: H. Subramaniasivam, Graduate Student
W. D. Lilly, Senior Technical Assistant

NIST Scientific Officer: Dr. G. W. Mulholland

Technical Abstract:

I. Thermophoretic Sampling of the Soot Formed In The Buoyancy Dominated Ethene, Methane and Acetylene Flames.
In the six months of this grant we have applied the thermophoretic sampling technique to unsteady buoyancy dominated flames that are formed when the flow rate is increased to 50 cm^3/s(1,2) using the above named fuels. The burner i.d. is 1.11 cm and a coannular air flow is provided. In the buoyancy dominated flame, which is well described in the literature, a toroidal vortex is formed near the height Z=15 cm above the burner. The vortex is shed aperiodically and breaks into a turbulent flame brush that extends to Z≈40 cm. The flame geometry is nearly identical for all three fuels but the ethene flame does display the stronger vortex action:

Ethene: Aggregates show systematic growth over the first 15 cm of the height Z where the vortex is located. At this height the primary particle diameter is approximately 35 nm. No further growth or oxidation of the aggregates is observed, and it is presumed that all soot generated is released to the surroundings. At the top of the flame there exists a smaller group of aggregates which have uniformly smaller primary particles. This smaller fraction of the total population is the result of either a reduced growth or partial oxidation. Low in the flame on the fuel side of the flame front, we find the substantial population of solitary, polydisperse particles, usually circular in cross section and often coexisting with young agglutinated aggregates. This important discovery is discussed further below.

Methane: Very small singlet particles are found in the lower part of this flame and these develop into aggregates with increasing height. The maximum diameter of the primary particles is observed to be about 35 nm. A moderate population of microparticles are found again on the fuel side of lower flame. These microdroplets precede the formation of carbonaceous soot. Unlike the ethene flame, the microparticles are found in the upper portion of the flame and some are probably released to the surroundings. The inception zone for methane is weaker but is expanded into the upper portion of the flame.

Acetylene: Intense formation of aggregates is observed even below the height Z=1 cm. Primary particle diameters range up to 45 nm. Microparticles are very dense in lower portion of the flame in the fuel rich region. The vortex region is noticeably weaker in the acetylene flame. A small population of microparticles is observed in the upper portion of the flame. All three of these fuels display an 11 to 15 hertz oscillation immediately below the vortex.

II. The Nature of the Microparticles.
The microparticles are better characterized by referring to tests conducted on the coannular laminar flame at Q=3.85 cm^3/s where extensive data now exists and by conferring with the related published literature:
1. Thermophoretic probing conducted on this flame at Z=10, 20, and 30 mm has revealed the existence of the microparticle field that has been previously found in the buoyancy dominated flames. The particle morphology along a given radial direction for prescribed height Z displays strong radial gradients in which 'transparent' microparticles are found on the fuel side, aggregates are found near the luminosity front, and small highly opaque singlets are found near the flame front. This morphology explains the paradoxical results reported by Santoro, Semerjian and Dobbins wherein at Z=15 mm [eta=0.061] it is found that the soot volume fraction and the maximum particle diameter are found at the same radial position as the minimum in soot number concentration. Coagulation theory would indicate that all three quantities should display a maximum at the same radial location. These counterintuitive results, which are also reported by Gomez et al. in their experiments on different fuels, have never been adequately explained. It now is apparent that the above described results are the outcome of using data analysis based on Rayleigh spheres on a particle field which has a strong gradient not only of morphology, but also of size distribution and refractive index as well.
2. Using the data for the above reference, we find the microparticle concentration to be 220 ng/cm^3, based on an assumed value of refractive index, at the radial position where the micrographs clearly display the presence of

microdroplets. A smaller imaginary component of the refractive index would result in a larger mass concentration.
3. The microparticles are found in the same regions where fluorescence was detected by Santoro and Semerjian. Since fluorescence is attributed to PAH species there is evidence that the microparticles are composed of mixtures of these materials.
4. Recently Feitelberg has shown that the total tar component of the PAH's is quantitatively correlated with the magnitude of the fluorescence cross section observed at 514 nm in response to laser stimulation at 488 nm. Tar was defined as the dichloromethane soluble fraction of the solid material collected from the atmospheric pressure premixed ethene flame in stainless steel probe. The fluorescence cross section observed of 1.4E-8 per cm-str yields a tar concentration in the ethene diffusion flame of 400 ng/cm^3 in approximate agreement with the above value found from the scattering/extinction measurements.
5. Wersborg et al. observed low opacity particles subject to coagulation in the lower portion of their low pressure premixed C_2H_2/O_2 flame. They made specific comment to the high contrast observed only in the case of the older particles and clusters higher in the flame. Their coagulating particles had volume mean diameters ranging from 1.5 to 15 nm. In this case the particles and gaseous species were collected by means of a supersonic nozzle. These observations are entirely consistent with our distinction between transparent coagulating microparticles and opaque aggregates.
6. Howard has recently described the formation of radical sites in PAH molecules, and the development of reactive coagulation of soot precursors. He also speculates that the heavy PAH's contribute the early soot growth. Our observations indicate that the soot particles are initially formed in the three flames observed above by the annealing at the flame front of the microparticles that are created in the fuel rich region.

III. Examination of Recent Laser Scattering/Extinction Tests. We presented the results of the reduction of existing laser scattering/extinction data using cross sections that we have formulated for polydisperse aggregates(3,4). Santoro, Puri and Richardson at Penn State have generated new laser scattering/extinction data for the nonsooting laminar ethene flame. This data has improved angular intensity measurements that permit the determination of the fractal dimension of the soot aggregate field. The results of this analysis provide strong support our previous description of the partitioning of soot dynamic processes in the laminar flame. An article is in

preparation on this topic(5). The above recent results on the presence and significance of microparticles does offer an important new understanding of the inception and growth processes of soot particles in diffusion flames.

Our presentation(6) on the interactive use of electron microscopy and laser scattering/extinction tests has been accepted for the annual meeting of the American Association for Aerosol Research at Traverse City in October 1991. The Principal Investigator was invited to participate in an international workshop at Heidelburg on Mechanisms and Models of Soot Formation commencing 30 Sept 1991.

IV. Impact of Research on Reducing Fire Losses:
A detailed knowledge of the evolution of soot provides data on the morphologies to be expected from evolving fires. The continued success of the work in predicting the optical properties of polydisperse soot aggregates improves confidence in the use these properties in fire detection and in fire research.

V. Reports and Publications:
1. Subramaniasivam, H., "Soot Formation in the Buoyancy Dominated Ethene Diffusion Flame", M. S. Thesis, Brown University, May 1991.
2. Dobbins, R. A., and Subramaniasivam, H., "The Evolution of Soot in the Buoyancy Dominated Diffusion Flames", Fall Meeting of the Eastern Section of the Combustion Institute, Ithaca, October 1991.
3. Dobbins, R. A., and Megaridis, C. M., "Absorption and Scattering of Light by Polydisperse Aggregates", Applied Optics, to appear October 1991.
4. Dobbins, R. A., Santoro, R. J., and Semerjian, H. G., "Analysis of Light Scattering for Soot Using Optical Cross Sections for Aggregates", 23rd Symposium (International) On Combustion, 1990 p1525.
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1.3 Turbulent Combustion

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - 1992

SIMULATION OF TURBULENT COMBUSTION AND TRANSPORT IN FIRES

Professional Personnel

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Hal C. Tang, CAML

Project Objective

To develop a fundamental understanding of the mechanisms which control the gas phase combustion and transport processes in fires and develop a predictive capability which will allow the computer simulation of these processes to be based on the mathematical expression of underlying physical principles.

Scope

A theoretical and computational approach to the study of the transport, mixing, diffusion, reaction, and radiation processes occurring in both enclosure and exterior fires. Emphasis is placed on gaining an understanding both of the individual phenomena, which occur on widely differing length and time scales, and on the interaction between them. Analyses and computer simulations of separate phenomena are combined and applied to problems of general interest.

Technical Accomplishments

Activities during FY 1991 focused on extending the enclosure fire transport computer simulation developed in earlier years in two directions; incorporation of a simplified combustion model into the large eddy simulation of fire induced flows, and allowing for the simulation of large fires in the open. Two closely related tasks were the evaluation and procurement of a new computer needed to perform the computations and the development of the eddy-scale combustion model to the point where it can be used to study the burning of real fuels. Each of these will be discussed in more detail below. An immediate application of much of this work is the oilspill burning project supported by the Minerals Management Service of DOI. It shares key technical components with the NASA supported microgravity ignition project.

The simplified combustion model incorporated into the two dimensional Navier-Stokes equation simulation of enclosure fire induced transport consists of assigning the heat release due to combustion to Lagrangian fluid elements representing fuel parcels convected with the large scale flow pattern. The model is mathematically consistent with the equations governing diffusion controlled combustion at large scales, exhibits the feedback associated with combustion, and permits the later incorporation of the eddy-scale combustion model currently under development into the large scale simulation code.

It makes use of the passive Langrangian smoke transport algorithm developed earlier, which is also used to visualize the transport of hot gases in fires. The extension of this capability to three dimensional flows is anticipated in the present fiscal year.

The extension to open environments consists of two parts: the analysis and implementation of boundary conditions "at infinity" in a rigorous and computationally tractable way; together with the inclusion of an ambient wind field as desired. The first of these tasks has been completed for the two-dimensional Navier-Stokes equation code. A similar analysis has been completed and implemented in three dimensions for the microgravity ignition project for the flow relevant to that problem. The mathematical problem is very similar in both cases, requiring the solution to an elliptic partial differential equation on a semi-infinite domain for every time step in the simulation. The computer codes for both problems implement boundary conditions derived from the use of the Greens functions for the relevant domains to calculated accurate conditions at the open boundaries of the computational space. This determines the pressure and the normal component of velocity, while the tangential component is determined from the condition that the fire induced flow away from the heated regions is irrotational.

The eddy-scale combustion model has been developed to the point where it can now be used for parametric studies of those fuels for which libraries of state relationships have been developed. At present data on seven fuels (H_2, CO, CH_4, C_3H_8, C_7H_{16}, C_2H_2, and C_2H_4) has been coupled to the generalization to three dimensions of the small scale mixing and diffusion model developed earlier. The model distinguishes between inviscid mixing of fuel and oxidizer by the combined action of strain and vorticity fields, and the molecular diffusion that lets the reactants come into close contact so that combustion can occur. The description involves many physical parameters whose relative importance must be assessed. This study, together with the development of an appropriate description of the role of soot and radiation at the eddy scale, will be a major activity in FY 1992.

The scale of the computations required to implement the analyses described above has grown as more physical processes and higher spatial and temporal resolution have been incorporated in the computer codes. This has led to a review of cost-effective computing resources that might be acquired to increase the capacity of the "computational combustion facility" shared with the Computing and Applied Mathematics Laboratory (CAML). After a series of benchmarking activities and studies of new and existing computer systems, it was decided that the purchase of an IBM RISC System 6000 model 550 to replace the existing Convex C120 computer made the most sense. The new system has 2.5 - 10 times the performance of the machine it is replacing, depending on which of our codes is run. It will have 256 Mbytes of memory and appropriate peripheral and networking capacity, permitting three dimensional simulations with over one million computational cells, a capability not feasible on the NIST central computer.

Publications

"Transient Combustion in a Turbulent Eddy", H.R. Baum, R.G. Rehm, and J.P. Gore, Twenty-Third Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, pp. 715-722 (1991).

"A Boussinesq Algorithm for Enclosed Buoyant Convection in Two Dimensions", R.G. Rehm, H.C. Tang, H.R. Baum, J.S. Sims, and D.M. Corley, NISTIR 4540 (1991).

Related Grants

"Fire Modeling", P. J. Pagni, University of California, Berkeley.

"Fire Propagation in Concurrent Flows", A. C. Fernandez-Pello, University of California, Berkeley.

"Radiation from Turbulent Luminous Flames", G. M. Faeth, University of Michigan.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution:	The University of California at Berkeley
Grant No:	GDOC 60NANB8D0848
Grant Title:	Fire Modelling
Principle Investigator:	Professor Patrick J. Pagni Mechanical Engineering Department 5131 Etcheverry Hall University of California Berkeley, CA 94720
Other Professional Personnel:	Javier J. Trelles (Ph.D. Candidate) Dr. Aruna A. Joshi Charles M. Fleischmann (Ph.D. Candidate)
NIST Scientific Officer:	Dr. Howard R. Baum

Technical Abstract:

Introduction. The overall goal of this project is to develop chemical, physical, and mathematical models of the detailed combustion phenomena which control a fire's growth. Our emphasis recently has been on pool fire coherent structures, window breaking in compartment fires, and backdrafts, i.e., the combustion of accumulated excess pyrolyzates. Since the Third IAFSS Symposium in Edinburgh, our glass breaking studies have focused on extending the program, BREAK1, to accommodate double pane windows. BREAK2, which will include a double pane option as well as improvements in the user interface, should be available in the Spring. Backdraft experiments by C.M. Fleischmann in collaboration with Professor R.B. Williamson are currently underway.

Vortex Shedding Experiments. To confirm the previously reported correlation of the annular coherent structure shedding frequency, f, with pool fire diameter, D, (see Fig. 1) additional experiments have been performed at Berkeley. Three fuels, of differing chemical structure, were burned in circular pans: methanol [CH_3CH_2OH], acetone [CH_3COCH_3], and iso-octane [$(CH_3)CHCH_2C(CH_3)_3$]. The pan diameters used varied from 4 to 100 cm. From a videotape of each run, the time period for shedding ~50 vortices was measured to determine a frequency. The results, averaged over several repetitions, are shown in Fig. 1 to be consistent with the correlation $f = 1.5/\sqrt{D}$. In addition, these videotapes will be utilized to provide comparisons with the analytical model of unsteady pool fire plume flow fields currently under development.

Flow Field Model. Rather than derive the fit shown in Fig. 1, we use it as a starting point to describe the inherently unsteady flow field associated with pool fires. We release a series of annular vortices with a period specified by the fit, along with their mirror to account for ground effects. Their circulations, $\kappa(t)$, and core radii, $\varepsilon(t)$, will be determined by matching time-averaged correlations for plume size and centerline velocities as given in Fig. Refs. 6 and 9. As a first step, the unsteady pure flow field generated by an ever increasing number of annular vortices and their mirror images is determined. The velocity field generated by a ring vortex of vorticity ω_ϕ can be obtained from the stream function equation

$$\frac{\partial^2\psi}{\partial z^2} + \frac{\partial^2\psi}{\partial r^2} - \frac{1}{r}\frac{\partial\psi}{\partial r} = -r\omega_\phi(r,z), \qquad (1)$$

where the radial and axial velocities are defined respectively as $ru_r = -\partial\psi/\partial z$, $ru_z = \partial\psi/\partial r$. The velocity components obtained form Eq.(1) are

$$u_r = \frac{\kappa a (z-b)}{\pi k^2}\frac{\left(-2F_1(k) + \frac{k^2-2}{k^2-1}E_1(k)\right)}{\left((r+a)^2 + (z-b)^2\right)^{3/2}} \qquad (2)$$

$$u_z = \frac{\kappa a\left(a^2 - r^2 + (z-b)^2\right)}{2\pi r\left((r+a)^2 + (z-b)^2\right)^{3/2}k^2}\left(-2F_1(k) + \frac{k^2-2}{k^2-1}E_1(k)\right) + \frac{\kappa\sqrt{a}}{4\pi r^{3/2}}\left(\left(\frac{2}{k} - k\right)F_1(k) - \frac{2}{k}E_1(k)\right) \qquad (3)$$

where $k = 4ar/\left((r+a)^2 + (z-b)^2\right)^{1/2}$ and $F_1(k)$, and $E_1(k)$ are the complete elliptic integrals of the first and second kind. Summing over the velocity fields of all previously introduced vortex ring pairs permits calculation of the current velocity field. The subsequent motion of each vortex core can then be calculated from this velocity field. To deal with the singularity in its own velocity field at the core of each vortex, an asymptotic expression for the self-induced axial velocity is used.

$$u_{zi} = \frac{\kappa}{4\pi b}\left(\ln\frac{8b}{\varepsilon} - \frac{1}{4}\right) \qquad (4)$$

Preliminary comparisons of experimental plume centerline velocities and shapes with the predictions from these equations to determine the appropriate values of $\varepsilon(t)$ and $\kappa(t)$, respectively, are underway.

Reports and Papers:

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2. Joshi, A.A., and Pagni, P.J., "Fire Induced Thermal Fields in Window Glass: I - Theory," submitted to *Fire Safety Journal.*

3. Joshi, A.A., and Pagni, P.J., "Fire Induced Thermal Fields in Window Glass: II - Experiments," submitted to *Fire Safety Journal.*

4. Joshi, A.A., "Fire Induced Window Glass Breakage," Doctoral Dissertation, Mechanical Engineering Dept., University of California, Berkeley, June, 1991.

5. Joshi, A.A., and Pagni, P.J., "User's Guide to BREAK1, the Berkeley Algorithm for Breaking Window Glass Times in Compartment Fires," and the program BREAK1 are available on the NIST Computer Bulletin Board.

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2. Byram, G.M., and Nelson, R.M., "The Modeling of Pulsating Fires," *Fire Technology*, 6, 102 - 110, 1970.

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14. Schoenbucher, A., et al., "Simultaneous Observation of Organized Density Structures and the Visible Field in Pool Fires," *Twenty-first Symposium (International) on Combustion*, The Combustion Institute, 1986, pp. 83 - 92.

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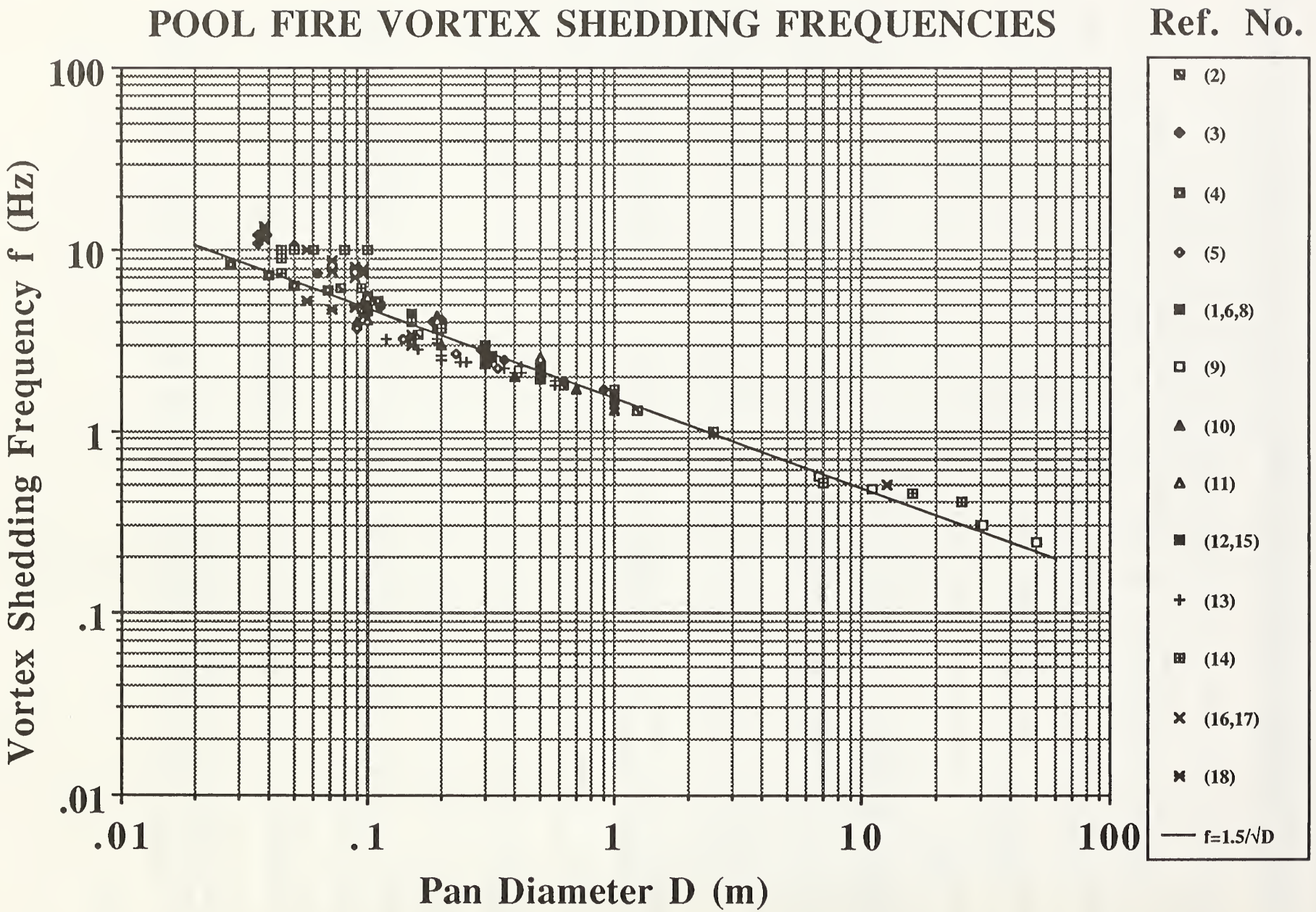
POOL FIRE VORTEX SHEDDING FREQUENCIES
Ref. No.
Vortex Shedding Frequency f (Hz)
100
10
1
.1
.01
.01
.1
1
10
100
Pan Diameter D (m)
(2)
(3)
(4)
(5)
(1,6,8)
(9)
(10)
(11)
(12,15)
(13)
(14)
(16,17)
(18)
f=1.5/√D

Figure 1.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 91

Institution:	University of California, Berkeley
Grant No.:	60NANB7DO737
Grant Title:	Fire Propagation in Concurrent Flows
Principal Investigator:	Professor A. Carlos Fernandez-Pello Department of Mechanical Engineering University of California Berkeley, CA 94720 Telephone: (415) 642-6554 Fax: (415) 642-6163
Other Professional Personnel:	Liming Zhou, Doctoral Student Christopher Chao, Doctoral Student
NIST Scientific Officer:	Mr. Kenneth Steckler

Technical Abstract:

An experimental study is being conducted of the effect of oxidizer gas flow turbulence on the concurrent spread of flames over the surface of a solid combustible. During this reporting year a research task has been completed to study the effect of air flow velocity and turbulence intensity on the burning of thick PMMA sheets in a ceiling configuration. The experiments included measurements of the concurrent flame spread rate, mass burning rate, flame length, surface heat fluxes, and combustion completion (CO, CO_2, HC), as a function of the flow conditions. The tests are conducted in a combustion wind tunnel already described in other progress reports, but with the fuel mounted in the ceiling of the tunnel test section. Tests were conducted with air flow velocities ranging from 0.25 to 4.5 m/s and grid induced turbulence intensities from 1% to 15%. The measurements show that the flow parameters affect significantly both the rate of flame spread and of mass burning, particularly at high flow velocities. The former increases with the flow velocity but decreases with the turbulence intensity, and the latter increases with both the flow velocity and the turbulence intensity. These trends are the result of the combined effect of the flow parameters on the surface heat flux and on the flame length. The flame spread rate measurements are correlated well with a simple expression derived from a heat transfer analysis of the problem. The mass burning rate data show that flat plate boundary layer analyses describe well the process, and a correlation of the data is obtained in terms of a nondimensional burning rate, and a flow parameter that includes the Reynolds number and the turbulent intensity. Comparison of the measurements for the floor and ceiling geometries show that buoyancy has an important influence in these process at least up to flow velocities of 5 m/s. Although for the same flow parameters both the flame spread and mass burning rates are larger in the ceiling configuration, the combustion is less complete than in the floor configuration. These results indicate that in the ceiling case buoyancy introduces two main competing effects, one is the enhancement of the heat transfer to the wall due to the reduction of the flame stand-off distance, and the other is the weakening of the combustion reaction due to wall quenching and reduced mixing of the pyrolyzate and air. A study is currently underway to study turbulent concurrent spread of flames in the ceiling and floor configuration under vitiated conditions.

Concurrent Ceiling Flame Spread. The measurements of the ceiling flame spread rate over PMMA sheets are presented in Fig. 1 for several air flow velocities and turbulent intensities. It can be seen that the flame spread rate increases with the flow velocity for all turbulent intensities tested, although the rate of increase is smaller for the larger turbulent intensities. These results agree qualitatively with the results from our previous experiments with the combustible in the floor configuration, and with boundary layer models of flame spread. As the flow velocity is increased, the boundary layer thickness decreases and the flame moves closer to the fuel surface, which enhances the heat transfer from the flame to the solid combustible, and as result, the flame spread rate. Fig. 1 also shows that the flow turbulence affects noticeably the ceiling flame spread rate, causing the spread rate to decrease for air velocities larger than 1 m/sec. This result is also consistent with the previous measurements on the floor configuration, and is the result of the shortening of the flame by the flow turbulence. However, for flows with velocities smaller than 0.75 m/sec, the flow turbulence has an opposite effect on the flame spread with the spread rate increasing slightly with the flow turbulence intensity. This trend, which differs from the results observed in the floor configuration seem to be related to the effect of buoyancy on the hot ceiling layer, which in turn affects the flame structure, and the rate of spread.

The Effect of Buoyancy on Concurrent Flame Spread. In Fig. 2, the flame spread rates from some of the floor and the ceiling experiments are presented together for comparison. Two turbulence levels of 1% and 15% are used to represent low and high turbulence cases, respectively. It is seen that for flows with velocities larger than 1 m/sec, the flame propagates faster in the ceiling configuration than in the floor case, which seems to be the result of enhanced heat transfer in the top case. The flame in the ceiling configuration is visually observed to be closer to the solid surface than that in the floor case, which is also confirmed by Schlieren images taken in different experimental conditions. In the ceiling case, the thermal boundary layer is thinner than the floor one and the flame is further away from the fuel surface. Hence, the temperature gradient from the flame to the solid surface becomes steeper and the heat transfer is enhanced, and the flame spread rate is increased. As the flow velocity is increased, the natural convection effect is expected to become less significant compared with the forced convection force. The measurements shows that for all turbulence intensity levels, the spread rate difference between the two cases becomes smaller as the flow velocity increases.

For the flows slower than 1 m/s, however, an opposite phenomenon is observed. The flame propagates slower in the ceiling configuration than in the floor case, contrary to the results obtained in flows with larger velocities. Obviously, other mechanisms other than the heat transfer one become more important under low flow velocity conditions. It is observed visually during the experiments that in the low flow velocity range, flames in the ceiling become very weak and display distinct blue color, unlike in those in the floor where yellow flames are always observed. It is known that the blue color is mainly emitted by the CO spectrum at low temperature and the yellow flames are caused by soot in the reaction zone at relatively high temperature. This observation suggests that the reacting zone in the ceiling configuration may be near extinction where chemical reactions are not complete, which results in a high CO concentration and a lower flame temperature.

To investigate the chemical kinetic conditions in the reacting zone, the exhaust gas concentrations of O_2, CO, CO_2, NO and unburnt hydrocarbons were measured under various flow conditions. Some typical results are shown in Fig. 3 for the flow condition of $U = 0.5$ and $u'/U = 1\%$. The gas concentrations are presented as functions of the pyrolysis front position for simpler comparison between the results for different cases. It is seen that that over most of the fuel surface much more CO and unburnt hydrocarbon are detected in the ceiling flame spread than in the floor one. Similar characteristics of exhaust gas concentrations have also been observed under other flow conditions of various flow velocities and turbulence levels. From these measurements, it can be concluded that for the flow conditions tested, the chemical reactions are less complete in the ceiling configuration than in the floor case. A good indication of

the completeness of the combustion is the unburnt hydrocarbon concentration. For the floor case the unburnt hydrocarbon is almost undetectable in all the flows including low flow velocity case. On the other hand, for the ceiling flame spread, the unburnt hydrocarbons are found in all flow conditions, even at velocities as high as 4 m/sec.

In the ceiling flame spread, buoyancy causes the hot fuel vapor to stay at the top, which deters its mixing with the cold air below and inhibits the completion of the combustion reaction. In the floor case buoyancy lifts the hot reacting gas, which enhances the mixing with the air above facilitating the completion of the combustion reaction. Another possible cause for the weaker combustion reaction in the ceiling spread is the quenching effect of the wall because the flame is pushed by buoyancy much closer to the fuel surface in this case. These results indicate that the ceiling flame spread takes place under local under-ventilated conditions while in the floor case the flame spreads under local over-ventilated conditions.

Mass Burning Rate. The surface regression rates for flow velocities U = 2 m/sec are presented in Fig. 4 for several turbulence intensity levels, as functions of the distance downstream from the flame leading edge. As seen in the figure, for all flow conditions the mass burning rates decrease with the downstream distance as a result of the thermal boundary layer growth. The flow turbulence also has an important influence on the ceiling mass burning process. Larger turbulence creates stronger eddy motions in the flow, which enhance the transport of heat and mass, and therefore increases the mass burning rate. However, the enhancing effect of the flow turbulence on the ceiling burning is not as strong as on the floor burning. The dependence of the surface regression rates on the flow velocity can also be seen from the data in Fig. 4. It is seen that as the flow velocity increases, the mass burning rate increases because the boundary becomes thinner and the flame is pushed closer to the solid fuel surface. The convective heat transfer is therefore enhanced and the mass burning rate is increased.

An attempt has been made to derive correlations for the non-dimensional mass burning rate and the flow parameters similar to the ones obtained for the floor burning rate. In this case the result of the correlation is less satisfactory. A possible reason is that the correlation is based on parameters derived from an analysis of the process that considers forced flow and infinitely fast kinetics, and as explained above these assumptions may not be totally valid in the ceiling burning case.

Reports and Papers:

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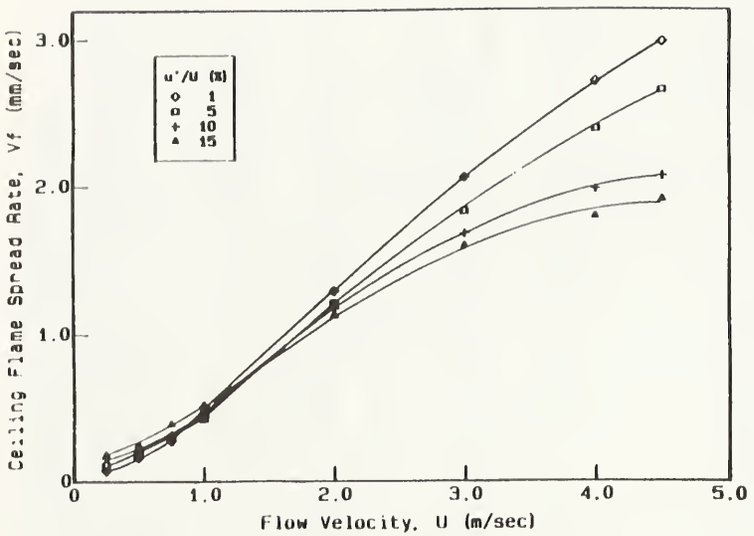
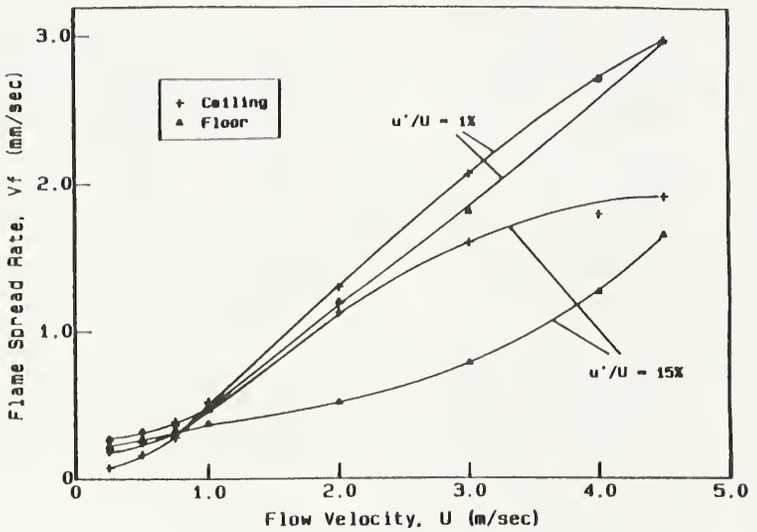


Figure 1.



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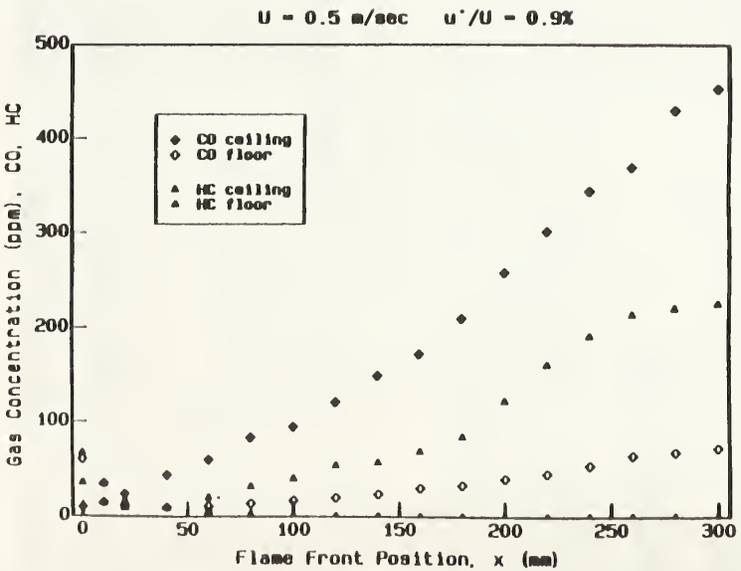


Figure 3.

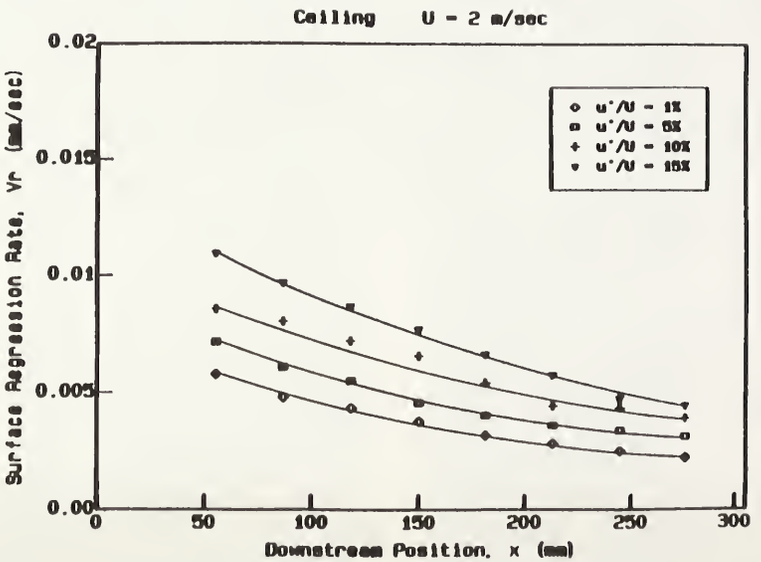


Figure 4.

1.4 Polymer Gasification

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - 1991

BURNING RATE

Professional Personnel

T. Kashiwagi, Project Leader
J. Brown, Chemist
A. Hamins, Mechanical Engineer
K. Steckler, Physicist
J.C. Yang, Post-Doctoral Fellow

Principal Objectives

(1) To improve our understanding of the physical and chemical gasification processes of various polymers and to develop theoretical models to predict the gasification rates of polymers exposed to fire conditions.

(2) To improve our understanding of energy feedback mechanisms of pool fires and to develop theoretical models to predict energy feedback rates from a pool flame to the fuel surface.

Scope

In order to accurately model the burning rates of polymers, both gasification rates and heat feedback rates from a flame to the fuel surface must be understood. Polymer gasification consists of three parts: thermal degradation chemistry, heat transfer and mass transfer processes in the polymer. Through a detailed study of each major component in the gasification process, a global model consisting of simplified sub-models will be developed. Flame heat transfer processes including heat feedback to the fuel surface are studied in a pool fire configuration. Pure liquid fuels are used to simulate the burning of polymer degradation products. A simple global energy feedback model is developed which takes into account fuel effects and the influence of pool diameter on the energy feedback rate.

Technical Accomplishments

I. Polymer Gasification

1. Experiments

An experimental apparatus for studying transient gasification of materials exposed to radiant heating in a nitrogen atmosphere is being completed. The apparatus includes a stainless steel water cooled chamber (0.6 m diameter and 1.5 m tall), a pneumatic lift for inserting the sample assembly into the

chamber, precision mass balance, radiant heater, and a water-cooled shutter located between the sample and the heater. Measurements will include temperature profiles within the sample, depth of bubble layer in the sample, and mass of the sample as a function of time.

2. Gasification Rate Model

A numerical surface-absorption model for the one-dimensional gasification of a non-charring thermoplastic material subjected to a constant external radiant heat flux was developed. The model assumes a one-step Arrhenius reaction at the surface. Figure 1 shows the results of this model compared with experimental results for PMMA. The pre-exponential factor was adjusted to obtain reasonable agreement between the theoretical and experimental results. Also shown in this figure are results from an earlier analytical model which assumes a constant vaporization temperature, T_v. The latter model produces an unrealistic jump in the mass-loss rate, whereas the model with the continuous Arrhenius reaction produces results that more closely follow the experimental data.

The next step is to expand the numerical model to include sub-surface degradation processes.

II. Pool Burning

1. Experiments

The energy flux at the surface of a pool fire was characterized. A narrow view angle (0.004 str or $\pm 7°$), nitrogen purged, water cooled radiometer was used to measure the radiative portion of the heat feedback to the surface of a 30 cm pool fire. Since the radiometer views only a limited portion of the flame, measurements were made radially from the pool center at 2 cm intervals and tilted at 20° intervals from 30° to 150° (normal to pool surface = 90°). The effect of gauge heat up was measured with the fire burning, by placing a water cooled cap over the radiometer (nitrogen purge maintained). The total radiative flux to the fuel surface at a particular location was calculated by numerically integrating the intensity profiles. The radiometer was calibrated using a standard flux gauge. The fuels tested were methanol (no soot), heptane (moderately sooting) and toluene (heavily sooting). These fuels were chosen because they yield flames with distinctly varying luminosities and heat release rates.

The total feedback to the fuel surface was calculated from fuel burning rates measured in a pool fire apparatus consisting of four concentric rings with the burning rate in each ring independently monitored. In addition, heat losses to the cooling water and increases in sensible heat of the fuel were determined to be small. Thermocouple measurements indicated that heat conduction from the flame to the fuel surface via the burner rim was negligible.

A comparison of the local radiative and total heat feedback for a 30cm methanol pool fire is shown in Fig. 2. The difference between radiative and total heat feedback is attributed to convection. Radiation is the dominant heat transfer mechanism occurring at the pool center, while convection is of importance near the pool edge only.

Measurements using oxygen calorimetry to ascertain combustion efficiency as a function of pool diameter and fuel type are being carried out. Additional flame radiance measurements are being planned for larger sized pool flames (diameter 0.6 and 1.0 m).

2. Burning Rate Model

A simple global model was developed which predicts the mass burning flux for pool fires consuming liquid fuels in a quiescent environment. The model assumed constant bulk properties such as flame temperature, soot volume fraction, and species concentrations. The computational procedure required knowledge of the fuel smoke point height and fuel properties such as the heat of vaporization, heat capacity, and boiling point. A cylindrical flame shape was assumed and the flame height was calculated using Heskestad's correlation. A mean beam length approach for radiative heat transfer was utilized and emission from both gas species and soot particles was considered. The convective heat transfer coefficient was estimated from Yumoto's pool fire measurements. Experiments in small pools were used to estimate conductive heat transfer. The predicted mass flux was within a factor of two of measured burning rates for pool diameters greater than 0.2 m and within a factor of three for smaller diameters. The global flame temperature was taken as the average of the maximum flame temperature and the fuel boiling point. The maximum temperature was based on the adiabatic flame temperature less the energy lost through radiation and combustion inefficiency.

Publications

"Analytical Model for Transient Gasification of Noncharring Thermoplastic Materials", Steckler, K.D., Kashiwagi, T., Baum, H.R., and Kanemaru, K., Third International Symposium on Fire Safety Science, Edinburgh, Scotland, 1991.

"Estimate of Flame Radiance via a Single Location Measurement" Hamins, A., Klassen, M., Gore, J., and Kashiwagi, T., Combustion and Flame, Vol. 86, 223-228 (1991).

"Fuel Property Effects on Burning Rate and Radiative Transfer from Liquid Pool Flames", Gore, J., Klassen, M., Hamins, A., and Kashiwagi, T., Third International Symposium on Fire Safety Science, Edinburgh, Scotland, 1991.

"Lip Effects in Liquid Pool Fires", Yang, J.C., Hamins, A., and Kashiwagi, T., submitted to Combustion Science and Technology.

"A Simple Model for Predicting the Burning Rate of Liquid Pool Fires", Hamins, A., Yang, J.C., and Kashiwagi, T., submitted to Fire Safety Journal.

Related Grants

"The Behavior of Charring Materials in Simulated Fire Environments", Eric Suuberg, Brown University.

"The Structure and Radiation Properties of Pool Fires", J.P. Gore, University of Maryland.

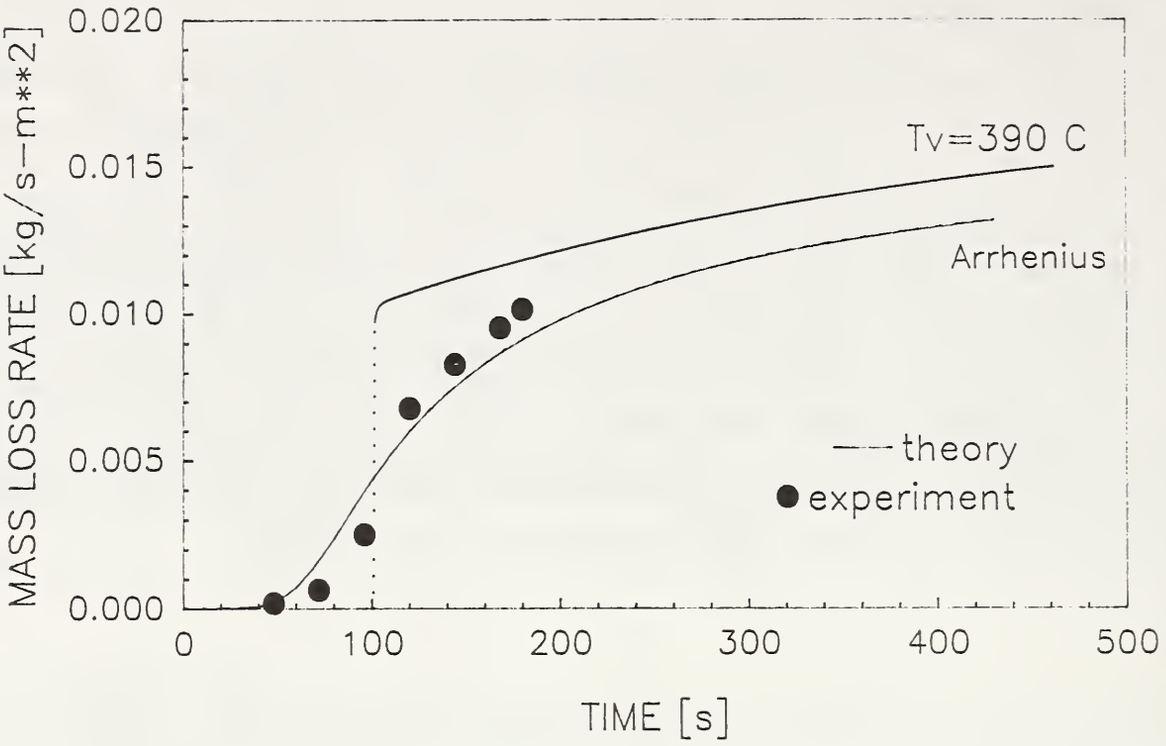


Fig. 1. Mass loss rate of PMMA exposed to 40 kW/m^2 incident heat flux.

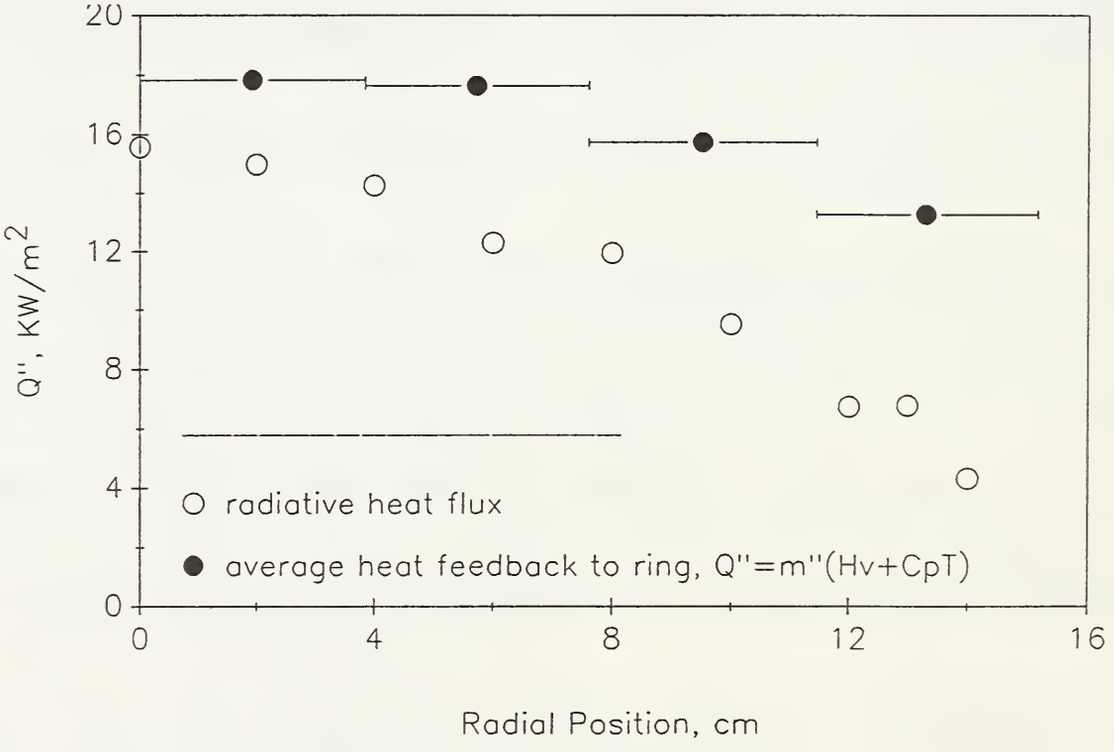


Fig. 2. Incident heat flux on the fuel surface as a function of ring number for various fuels in a pool fire apparatus.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 91

Institution:	Brown University
Grant Number:	60NANB0D1042
Grant Title:	The Behavior of Charring Materials in Simulated Fire Environments
Principal Investigator:	Prof. Eric M. Suuberg Division of Engineering Brown University Providence, R.I. 02912 (401) 863-1420
Other Professional Personnel:	Mr. William Lilly, Senior Research Engineer Mr. Ivan Milosavljevic, Student
NIST Scientific Officer:	Dr. Thomas Ohlemiller

Technical Abstract:

Introduction. The complicated interplay of chemistry, heat and mass transfer serves to make the study of combustion phenomena generally quite difficult, particularly when a solid phase is also involved. If the solid phase consists of an organic macromolecular material, the complexity is compounded by the need to account for a host of pyrolytic phenomena in addition to the gas phase processes. This is unfortunately the situation in study of fire phenomena.

The general topics that are of concern in this project include:

1. Detailed kinetic models will not be soon developed for most cases of practical interest, so there is a question as to whether approximate methods can capture the essence of the processes. In particular,there is concern about when small scale laboratory pyrolysis data can be reliably used to model fire situations.
2. Within the above framework, can the rates of release of certain types of toxicants be predicted?
3. How does the composition of volatiles affect flammability, fire luminosity and smoke

The primary emphasis in this project is in area 1.

A more complete understanding of the processes that determine yields of volatiles and char in solids pyrolysis can still play a pivotal role in the specification of conditions that mitigate hazardous conditions.

Considerations in Performing Pyrolysis Studies of Relevance to Fire Modeling Any study of fire phenomena that involves the study of chemistry in an environment that is removed from that encountered in actual fire situations runs a significant risk of producing results that do not accurately model actual fire behavior. This is not to deny the value of model studies, for these are undoubtedly of great value in advancing fundamental understanding of many aspects of the problem; the concern is in our ability to predict a priori the key variables that must be controlled in order to accurately simulate conditions of relevance. Studies of pyrolysis of organic solids have been performed under an enormous variety of conditions, and the question

in the fire literature has been often raised as to which if any of the studies are of relevance to fire modeling? It seems wise in situations in which the entire variable set that might affect fire chemistry behavior has not been well established, to employ an approach that combines the examination of behavior in real fire situations with more controlled laboratory experimentation. This is the guiding philosophy of the present study.

The actual focus of the present work is on the behavior of charring solids during combustion in a fire environment. Wood and many synthetic polymers, particularly those that are crosslinked, fall into this class of materials. Obviously this is a class of some significant practical interest. It has been reported that the char forming tendency of organic materials may be predicted from a knowledge of their chemical structures (e.g. Van Krevelen, Polymer, 16, 615 [1975]), and that this char forming tendency is correlated with the limiting oxygen index (LOI). There are of course some significant questions about the relevance of the LOI itself as an indicator of fire behavior, but still the possibility of predicting features of some relevance to the behavior of the material in a fire environment from chemical structure alone, is significant. It should however be remembered that the char forming tendency of a material may be affected by factors other than the chemical structure of the polymer itself. The yield of char in cellulose pyrolysis has, for example, been reported to be a function of impurity or retardant content and of heating rate (although recent work in this laboratory has revealed only a minor effect of this variable , in the absence of transport limitations).

The role of a char layer in complicating the analysis of the combustion process has been recognized by many workers in the field. The char has a high emissivity and may thus participate in mechanisms of extinguishment by heat loss from the surface. If not screened by the outward flux of volatiles, the char may itself react with oxygen, and become a local heat source, as in glowing combustion. The char may also be highly catalytic in promoting cracking reactions of volatiles, changing the composition of the volatiles from that which exists in the active pyrolysis zone. The cracking may also result in additional carbon deposition in the char layer. If the volatiles contain carbon dioxide or water vapor and the char temperature is high enough, some gasification reactions may occur, resulting in release of hydrogen and/or carbon monoxide from the char. Such possibilities have been often recognized, but generally not studied in a systematic manner. A significant difficulty in performing such studies in a controlled environment is that the mass transfer in the char layer is imperfectly understood. For example, in real fire situations, wood forms a char layer with a partially crazed (alligatored) surface, and that suggests the possibility of cracks carrying volatiles out from below the char layer. This means that the residence time of the volatiles in the char layer (or extent of contacting between the two) is unknown, and thus difficult to quantitatively model. This aspect is the first to receive significant attention in this work.

Experimental Approach There is a need to tie the impressive progress that has been made in measuring and predicting char yields from pyrolyzing organic solids under laboratory conditions to predicting the yield under actual fire conditions. The particular approach employed here involves the use of equipment that has been developed to simulate the environment of real wall fires. The device was earlier extensively utilized in Center for Fire Research supported work on the combustion properties and behavior of pure and fire retarded cellulose, under the direction of Professor M. Sibulkin of Brown University. The actual device is shown schematically in Fig.1. It can be seen to have some similarity to apparatus used by workers at Factory Mutual Research Corporation for studies on flammability of plastics (Tewarson and Pion, Comb. and Flame, 26, 85 [1976]), except that the present device is intended mainly for studies on the pyrolytic behavior of the solid samples, rather than for studies on flaming combustion.

Briefly, the equipment allows bulk samples of several centimeter diameter and length to be held in an insulating ceramic holder atop an electronic balance. The assembly is held in a controlled gas environment, which can be purged with either nitrogen or nitrogen containing some low levels of oxygen. The environment can then simulate either a diffusion flame

environment, in which little or no oxygen reaches the surface of the sample, or a pre-ignition environment, in which pyrolysis begins in the presence of oxygen and a radiative flux from a fire elsewhere in the environment. The sample surface is heated by radiant quartz heaters which can provide a flux of up to about 100kW/m^2, which should cover the range of relevance in fire situations (somewhere around 40kW/m^2 is a "standard" condition).

The windows of the system are designed to permit the radiant heating of the sample as well as viewing of the sample, photography of the surface in real time, and pyrometric determination of the surface temperature of the sample. The sample itself can be instrumented within its interior with thermocouples, to provide a temperature profile, and the surface temperature can also be measured optically. We can determine the emissivity of the char in-house, using diffuse reflectance techniques on a FTIR spectrometer.

The yield of volatiles is provided by the data on mass loss of the sample. The analysis of the volatiles is provided by gas chromatography. The analysis by GC provides information only on the gaseous species, and the tars must be separately collected by condensation, or determined by difference. The apparatus is as of this writing being used to assess the effect of a char layer on volatiles composition.

In addition to the equipment described above, this laboratory also has available a separate pyrolysis reactor system that permits the examination of pyrolysis behavior of thin samples at heating rates that may be varied between 1°C/min and 1000°C/sec. This device has the advantage of providing the ability to examine the charring behavior in an environment free of mass transfer limitations. The pyrolysis is actually performed in a wire gauze which serves as both sample holder and electrical resistance heating element. The gauze is contained within a chamber in which the gaseous environment can be controlled. The heating rate of the sample is controlled by a thermocouple sensor-computer controller circuit. This device will provide a benchmark value of char yield and volatile product composition, against which to compare the results from the fire simulation experiments.

Results Obtained Work thus far completed has involved examining in detail the pyrolysis behavior of high density cellulosic samples. These samples have densities approaching those in wood (about 1 g/cc), but have the advantage of uniform, known composition and low impurity levels. The samples are pressed in house from cellulose pulp. The tests performed under nitrogen (with a surface radiative flux of 40 kW/m^2) in the simulated fire apparatus of Fig. 1 displayed the expected behavior, involving progressive penetration of a thermal wave into the sample. The residual "char" yields from such experiments were in the neighborhood of 10 to 20%, by mass. The term char is operationally defined as what is left behind as solid, following about one half to one hour of heating. In thin samples (a few mm thickness), the char was rather uniform in nature, and was quite black. In thicker samples, the char at the rear of the sample was brown, and obviously not as severely pyrolyzed; the char layer ahead of it had effectively insulated this material, so that even at final steady state, it was not fully pyrolyzed. This shows the danger in simply reporting "char" yields in fire situations. The chars may in fact be quite different in character (e.g.potential for further pyrolysis if conditions change, reactivity in smolder situations).

It was noted in this work that the alligatoring behavior commonly seen in wood could be suppressed or enhanced, depending upon sample configuration. Alligatoring involves the macroscopic cracking of the sample, due to shrinkage during pyrolysis. Allowing small samples to shrink inward during pyrolysis largely prevents alligatoring, whereas confining the edges of a sample to prevent inward shrinkage, causes cracking failure in the middle of the sample. It was observed in the process of studying this phenomenon that the effective flux of volatiles in the high density samples was parallel to the surface of the sample, in a direction normal to the incident radiative flux. The volatiles would often apparently flow a much longer distance in the direction parallel to the face of the sample than flowing a short distance through the front face. Thus alligatoring cracks potentially serve as important conduits of volatiles, and

an assumption of uniform surface flux of volatiles may be rather poor in some situations. A striking demonstration of the effects of non-uniform permeability is provided in Fig. 2, from experiments performed on the same materials in the heated wire mesh apparatus described above. Rectangular samples of 2.7 mm thickness and 27 mm length were heated uniformly on both sides in the wire mesh. The yield of char was rather sensitive to the width of the wafers, as can be seen from Fig.2. This is presumably because the longer the distance that the volatiles need to flow to reach the thin edge of the sample, the more opportunity for cracking reactions to occur (cracking reactions lead to more char deposition). This phenomenon is certainly sensitive to sample density, anisotropy related to pressing, and possibly to the temperature history of the sample surface. The relative importance of these effects is being explored at present.

Emphasis is turning towards the composition of the volatiles. As a first step, attention is being directed at characterizing the principal tarry volatiles of cellulose pyrolysis. From the perspective of characterizing correctly the escape of these materials from the pyrolyzing cellulose, the vapor pressures of these materials are of interest. While compositional analysis and molecular weight analysis of the materials are under way, initially a more operational characterization was performed. Tars from the simulated fire apparatus were placed in the heated wire mesh apparatus and reheated at rates comparable to those seen by the bulk sample (60°C/min). Results are seen in Fig. 3. The tars show a continuous vaporization curve between about 200°C and 300°C, crudely corresponding to an ordinary boiling point curve, except that the backpressure on the tars is low. This shows that under ordinary pyrolysis conditions, the tars that escape during the most active phase of pyrolysis (above about 450°C) are not limited in their evolution by volatility. Rather, it is the rate of their formation by reactions that determines when they can escape. The potential for cracking reactions to influence what is seen in the volatiles is also evident in Fig. 3. It can be seen that the tar is not fully revaporized. Some of it is cracked, during the heating regimen, and forms a non-volatilizable residue. This aspect of the problem will also receive further attention.

Reports and Papers This project is at present nearing the end of its first year. No formal papers have yet been published from this work. It is expected that a submission will shortly be made to a section meeting of the Combustion Institute and possibly to the annual meeting of the Institute this coming year.

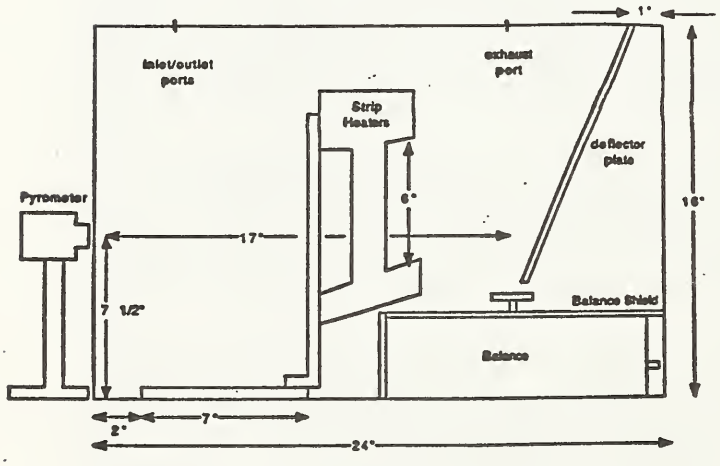
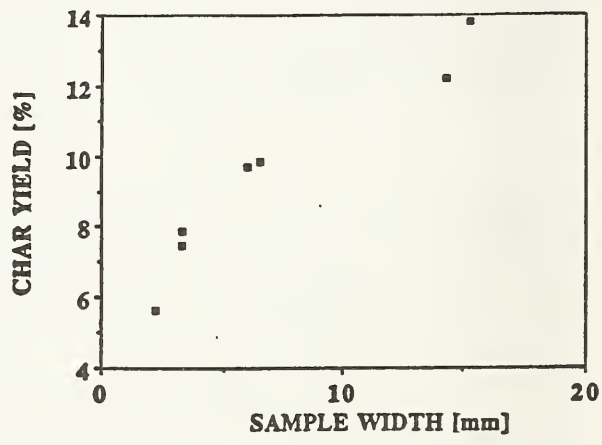
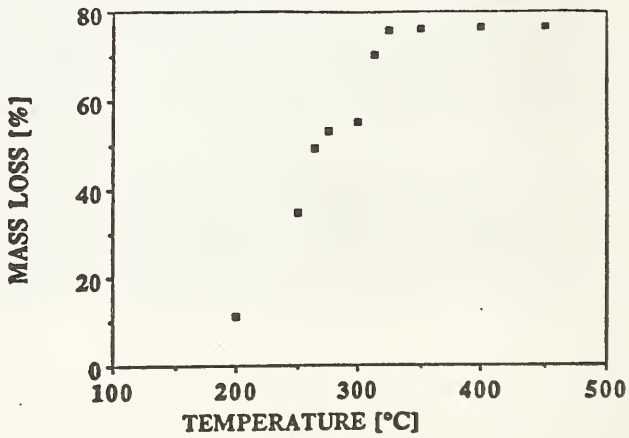


FIGURE 1: RADIATIVE HEATING SYSTEM



Top right Figure 2. Effect of sample wafer width on char yield.



Bottom right Figure 3. Vaporization of cellulose tars from a wire mesh heated at 60°C/min.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution: University of Maryland

Grant No: 60NANB9D0944

Grant Title: A Study of Structure and Radiation Properties of Pool Fires

Principal Investigator: Dr. J. P. Gore
Mechanical Engineering Department
University of Maryland
College Park, MD 20742

Other Personnel: Mr. M. Klassen, Doctoral Student
Dr. Y. Sivathanu, Research Associate
Mr. J. Chen, Graduate Student

NIST Scientific Officer: Dr. Takashi Kashiwagi

Technical Abstract:

Introduction: Burning rates of objects on fire determine safe egress times, heating rate of surrounding objects and flame spread rates. Radiative heat flux from fires to surrounding objects determines the possibility of ignition, flame spread and flashover. Improved understanding of phenomena that determine the burning rates and radiation loading of pool fires when incorporated into design and emergency management procedures can reduce fire losses.

The present project is designed to address the following unanswered questions involving heat feedback and radiation loading to the surroundings: (1) radiative component of the heat feedback for various fuels and pool sizes; and (2) effects of turbulent fluctuations on the mean heat feedback and radiation loading

(1) Radiative Component of the Heat Feedback: In the past the relative importance of radiative and conductive (including convective enhancement) components of the heat feedback have been determined for few fuels using plots of burning rates with pool diameter. For diameters greater than a certain limit, the feedback is expected to be dominated by radiative heat transfer. Naturally, the diameter at which the fire becomes dominated by the radiative heat feedback, depends on the fuel type mainly through its sooting tendency. Similarly, at different locations on the pool surface the fraction of radiative heat feedback is expected to be different.

Past measurements of local radiative and convective feedback have relied on Gardon gauges with different surface emissivities. However, coating of the surfaces with soot particles, variations in convective component due to changes in gauge surface temperature

introduce uncertainties in these data. In order to avoid these difficulties, a narrow angle radiometer was used to obtain the total directional heat feedback at different radial positions in 30 cm pool fires. Three fuels, methanol- representing nonluminous behavior, heptane- representing a moderately sooty fire and toluene -representing a heavily sooty composition were studied. Measurements were completed for 8 orientations covering the hemispherical view and the total radiative feedback was obtained using a weighted addition of the directional heat fluxes. Measurements were completed at multiple radial locations on the fuel surface.

Figure 1 shows a plot of the measured radiative heat feedback for methanol, heptane and toluene fires burning in a 30 cm pool. Comparison of these data with the local burning rate data obtained from a multi-ring pool fires and with measurements using a Gardon gauge shows that the feedback for all three fuels is entirely dominated by the radiative component at the centerline. This is somewhat unexpected in view of the nonluminous nature of the methanol fire. However, it appears that the low convective coefficients at the centerline combined with the long optical paths near the center lead to large contribution from radiation. Near the edge, the feedback becomes increasingly convective. For the heptane and toluene fires, the heat feedback is close to 100% radiative near the center. For heptane fires, the radiative component decreases to 75% near the edge. However, the toluene fires are dominated by radiation at all points on the surface. Past measurements of heat feedback using the two-emissivity Gardon gauges for 30 cm heptane fires had shown approximately 65% radiative contribution at the center. In view of the present data and the uncertainties of the two-gauge technique, the radiation dominated limits of fires are being reexamined.

In order to estimate the radiative feedback to the fuel surface using distributions of scalar properties in the fires, a five-line emission absorption probe is being used to obtain local measurements of soot volume fractions (for toluene and heptane fires), temperatures and CO_2 concentrations. Attention during the last year was focussed on toluene fires, since bulk of the radiative heat flux from these originates from soot particles. Measurements in 7.1 cm and 30 cm fires have revealed that bulk of the soot particles in the fire are at temperatures too low to significantly contribute to the radiative fluxes. This observation explains the lack of sensitivity of X_R to the sooting tendency observed in early part of the present study. Large intermittency in temperatures and soot volume fractions were also observed at all locations in the pool fires.

The transient data concerning the temperatures and soot volume fractions were used in conjunction with a new radiation model to predict the heat feedback to the fuel surface. The radiation model utilizes mean values of products of Planck function and absorptance of a path rather than the mean temperatures and soot volume fractions. The segments of the radiation path are chosen such that

the intensity leaving one segment is not correlated with the transmittance of the next segment. With this model, the computationally intensive procedure involving random simulations and simultaneous field measurements of scalars are avoided. However, the model accounts for the effects of turbulence-radiation interactions reasonably well.

Figure 2 shows predictions of radiative heat feedback for a 7.1 cm toluene pool fire obtained from multi-ray calculation utilizing the new radiation model (labelled Stochastic). Results of the conventional procedure involving the use of average temperature and soot volume fractions are shown for reference. These are lower by a factor of 10 compared to the new radiation procedure that accounts for the effects of turbulent fluctuations. Similar calculations are in progress for the 30 cm pool fire and early results for the feedback near the center are promising.

Future work will involve continued evaluation of the multi-ray PDF feedback calculation procedure for radiative heat feedback. Measurements of X_R and burning rates for 1 m and larger pools are planned in collaboration with the Fire Research Institute of Japan. Development of new global model is being supported by the detailed measurements and multi-ray predictions

Acknowledgement: The contributions made by Dr. Anthony Hamins of N. I. S. T. are gratefully acknowledged.

Reports and Papers:

1. J. P. Gore, M. Klassen, A. Hamins and T. Kashiwagi, "Fuel Property Effects on Burning Rates and Radiation Transfer Properties from Liquid Pool Fires," Third International Symposium on Fire Safety Science, Edinburgh, Scotland, 1991.
2. J. P. Gore, M. Klassen, A. Hamins and T. Kashiwagi,"Effects of Fuel Properties on Burning Rates and Radiation Properties of Pool Fires," Twenty Third International Symposium on Combustion (Poster Session), , 1990.
3. J. P. Gore and M. Klassen, "A Study of Structure and Radiation Properties of Pool Fires," Annual Report under Grant No. 60NANB09D0944, The University of Maryland, Mechanical Engineering Department, College Park, MD.
4. A. Hamins, S. Fischer, Kashiwagi, T., J. P. Gore and M. Klassen, "Measurement of Heat Feedback in Liquid Pool Fires," Combust. Sci. Tech., revised, 1991.
5. A. Hamins, M. Klassen, J. P. Gore and T. Kashiwagi, "Estimate of Flame Radiance via a Single Location Measurement," Comb. Flame, in press.
6. A. Hamins, M. Klassen, J. P. Gore and T. Kashiwagi, "Measurements of Radiation Feedback to a Pool Fire Fuel Surface," Proceedings of the Twenty-third Fall Technical Meeting of the Eastern States Section, The Combustion Institute, Orlando, FL, pp. 58.1-58.4.
7. M. Klassen, A. Hamins, J. P. Gore and T. Kashiwagi, "Heat Flux to the Surface of a Pool Fire," Proceedings of the Twenty-Fourth Fall Technical Meeting of the Eastern States Section, The Combustion Institute, submitted.

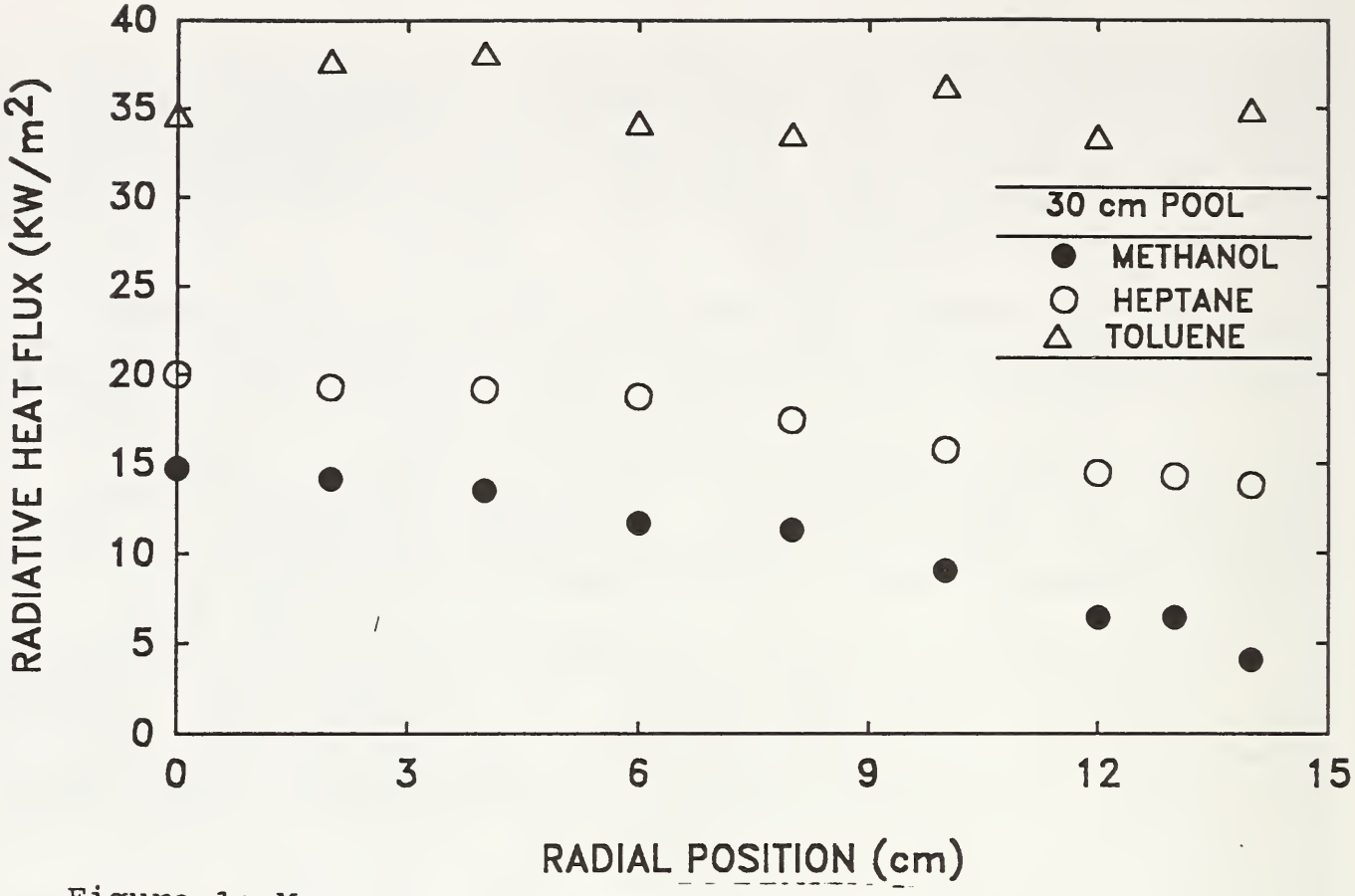


Figure 1: Measurements of Radiative Heat Feedback for 30 cm Pool Fires

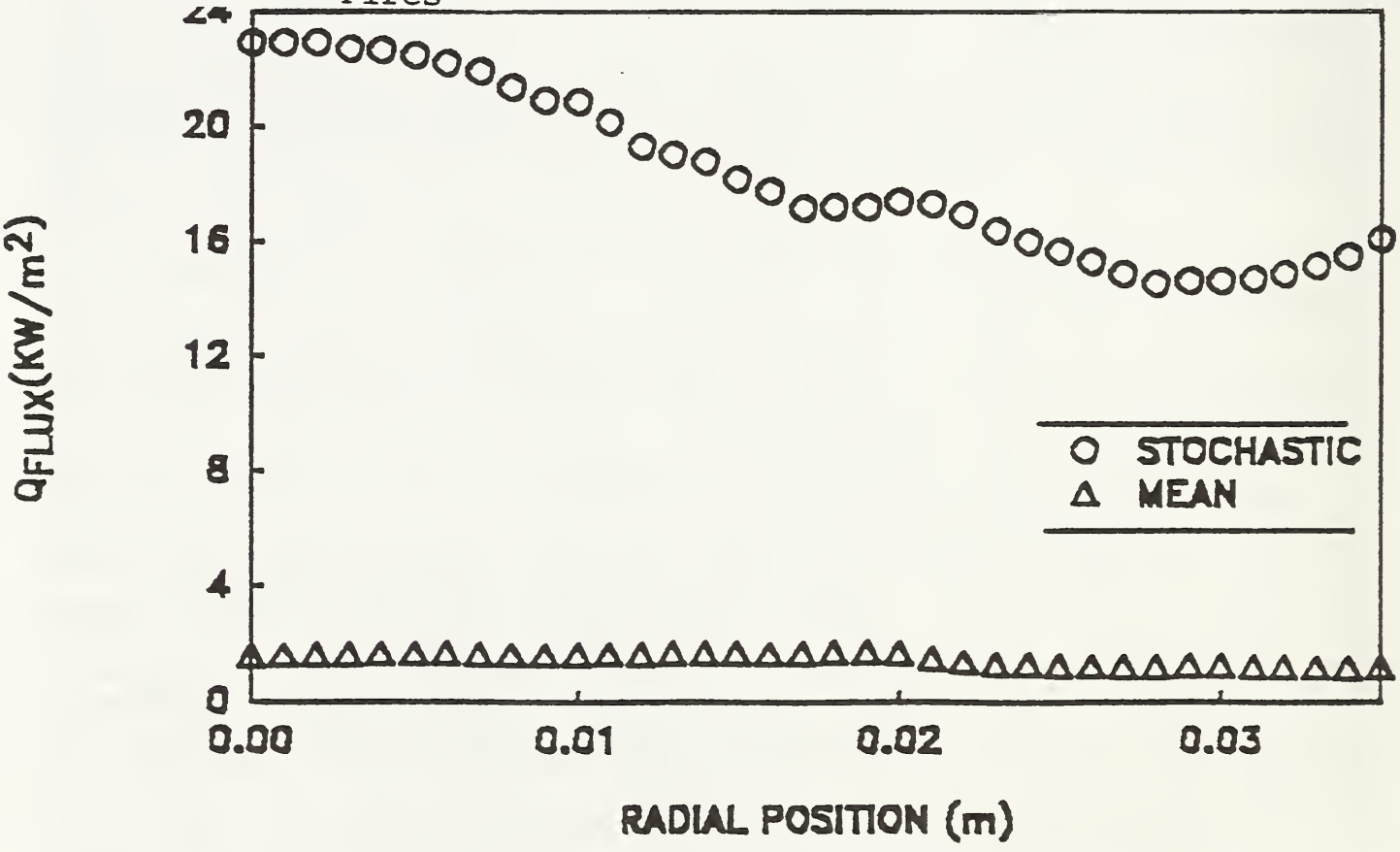


Figure 2: Calculations of Radiative Heat Feedback for 7.1 cm Toluene Fire

1.6 Toxic Potency

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT – 1991

TOXIC POTENCY MEASUREMENT

Professional Personnel

Vytenis Babrauskas, Group Leader
Barbara C. Levin, Toxicologist
Maya Paabo, Research Chemist
Emil Braun, Physicist
Richard H. Harris, Jr., Chemist
Magdalene Navarro, Biologist

Project Objective

To provide by July 1991 a rational and practical system for obtaining accurate toxic potency data for hazard models and product evaluation; to predict toxic effects of fire gases on rodents and humans.

Technical Approach

1. Various materials will continue to be explored in the new radiant heat system, in an effort to discover and set right any points of weakness.

2. Prepare a protocol for use of the bench-scale data in predicting real-scale performance.

3. A writeup of the test procedure will be provided in ASTM format.

4. Experimental work needed to complete N-gas model and to include NO_2 into the model will be completed.

5. The modified CFK equation for CO prediction will be documented against NIST rat data and against literature human data.

Technical Accomplishments

During this past year the development of the new radiant system for toxic potency testing was completed. The study results on this will be published very shortly. The validation of the method rests on data already collected during FY90 studies, a current short-term validation project to be completed by the end of FY91, and a final validation study to be done during FY92. The method has been drafted in ASTM format and submitted to the ASTM task group.

This study is the principal product of a research program to provide a technically sound methodology for obtaining and using smoke toxicity data for hazard analysis. It establishes:

(a) an improved bench-scale toxic potency measurement, one which represents the important combustion conditions of real fires;

(b) the feasibility of using the N-Gas Model for predicting the toxicity of combustion products under both bench-scale and full-scale testing; and

(c) a design and analysis framework which will allow the toxic potency data to be used in a rational, consistent, appropriate, and adequate way.

This establishment of proper bench-scale test conditions, validation of the output against real-scale fire measurements, and development of a consistent framework for fire hazard analysis is unique and represents a successful, usable implementation of the state of the art.

The experimental work necessary to include NO_2 into the N-Gas Model was completed and presented in part at the annual meeting of the Society of Toxicology.

Progress was also made on pharmacokinetic modeling during FY91. Both additional rodent data were collected and consolidations of governing equations was accomplished. The model now also allows the modeling of human CO uptake and elimination, based on literature values of the needed respiratory and blood gas constants.

During this year, some aspects of our studies were partially funded by the Society of the Plastics Industry, Inc.

Reports and Publications

Babrauskas, V., Harris, R.H., Jr., Braun, E., Levin, B.C., Paabo, M., and Gann, R.G., Large-scale Validation of Bench-scale Fire Toxicity Tests, J. of Fire Sciences. Vol. 9, 125-149 (1991).

Babrauskas, V., Levin, B.C., Gann, R.G., Paabo, M., Harris, R.H. Jr., Peacock, R.D., Yusa, S., Toxic Potency Measurement for Fire Hazard Analysis. Manuscript in review.

Levin, B.C., Paabo, M., and Navarro, M., Toxic interactions of binary mixtures of NO_2 & CO, NO_2 & HCN, NO_2 & reduced O_2, AND NO_2 & CO_2. The Toxicologist, Vol. 11, 222 (1991).

Babrauskas, V., Harris, R.H. Jr., Braun, E., Levin, B.C., Paabo, M., and Gann, R.G., The role of bench-scale test data in assessing real-scale fire toxicity. NIST Technical Note 1284, National Institute of Standards and Technology, Gaithersburg, MD, January, 1991.

Levin, B.C., Progress Report on Fire Toxicity and Chemistry Research in the United States. Eleventh Joint Panel Meeting on Fire Research and Safety, NISTIR 4449, Ed. by N.H. Jason and D.M. Cramer, National Institute of Standards and Technology, Gaithersburg, MD, pp. 64-69, October, 1990.

Related Grants

"The Effect of Oxygen Concentration on the Evolution of Toxic Gases from Douglas Fir, Rigid Polyrethane Foam and PVC," Arthur Grand, Southwest Research Institute.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution:	Southwest Research Institute
Grant Number:	60NANBOD1056
Grant Title:	The Effect of Oxygen Concentration on the Evolution of Toxic Gases from Douglas Fir, Rigid Polyurethane Foam and PVC
Principal Investigator:	Arthur F. Grand, Ph.D. Southwest Research Institute Department of Fire Technology 6220 Culebra Road P.O. Drawer 28510 San Antonio, Texas 78228-0510
Other Professional Personnel:	Walter G. Switzer, M.S.
NIST Scientific Officer:	Dr. Vytenis Babrauskas

Technical Abstract:

Summary. Combustion and gas analysis studies were conducted using the SwRI laboratory radiant combustion and exposure apparatus at a heat flux of 50 kW/m^2. The purpose of these studies was to determine the effects of ambient oxygen (O_2) concentration on certain gaseous products of combustion of three polymeric materials, Douglas fir (DF), rigid polyurethane foam (RPU) and polyvinyl chloride (PVC). Of particular concern was the evolution of the toxic gases carbon monoxide (CO), hydrogen cyanide (HCN) and hydrogen chloride (HCl). The results of this program have helped define the appropriate conditions under which this apparatus is suitable for laboratory studies involving combustion, gas analysis, smoke toxicity and smoke corrosivity. One of the conclusions reached was that selection of specimen sizes must be done with careful consideration of the resultant oxygen concentration (i.e., oxygen depletion due to combustion), in studies where different materials will be compared. The transition from flaming combustion to nonflaming combustion, which can cause a dramatic change in the yield of CO, may be affected by the O_2 concentration. The yields of HCN and HCl were less influenced by changing oxygen conditions in these experiments.

Test Program. The apparatus used for these studies is pictured in Figure 1. It consists of a quartz combustion cell and a clear plastic exposure chamber, which are connected by a stainless steel chimney. The specimen is located within the combustion cell on a platform connected to a load cell for continuous monitoring of mass. The heat flux, measured at the surface of the specimen, is supplied by tungsten-quartz radiant heat lamps, which are situated outside the combustion cell. A spark igniter provides a source of ignition. Smoke from the specimen, due to pyrolysis or combustion, travels up through the center section of the chimney into the exposure chamber. Air from the exposure chamber (which becomes vitiated as the combustion proceeds) is drawn down through the outside sections of the chimney by a heat pump effect into the combustion cell. Thus, the combustion zone has the same concentration of O_2 as in the exposure volume. At the end of the "irradiation time" (i.e., the combustion

time), the smoke shutter is closed in order to prevent any further smoke from entering the exposure chamber.

The oxygen concentration in the exposure chamber (and thus in the combustion cell) was established prior to any combustion of the specimen by metering nitrogen into the enclosed volume. Once it was verified that the oxygen concentration was at the target concentration, the combustion was initiated by activating the heat lamps and the spark igniter. The oxygen level was then maintained as close as possible to the initial reading by metering pure O_2 into the exposure chamber during combustion.

Specimens of the selected materials were evaluated at two different sizes (26 cm^2 and 52 cm^2 surface area) and at a single heat flux (50 kW/m^2). Oxygen concentrations ranged from 14 to 21 percent.

Results. Oxygen concentration affected the mode of burning in these studies (i.e., flaming vs. nonflaming), which in turn influenced the evolution of carbon monoxide (CO). This was not an unexpected observation, but one worth documenting because it has implications for the proper operation of this apparatus and because these effects could bias the results obtained. Yields of HCl and HCN were not substantially affected by the O_2 concentrations in these experiments; however, other products of pyrolysis and combustion, such as partially oxidized hydrocarbons could have been affected. These hydrocarbon species were not measured in this study.

Figure 2 is an illustration of the pattern of CO concentration and CO yield for one of the experiments involving Douglas fir (this run was conducted with a 52 cm^2 specimen at 16 percent O_2). During the flaming period (up to about 16.5 min.), the evolution of CO was low, as evidenced by both the concentration and the yield plots. Relatively little CO was released during most of the flaming portion of the test run (the small peaks and valleys correspond to changes in the intensity of the flaming). However, the transition to nonflaming combustion produced a dramatic increase in the yield of CO (approximately 30-fold in this case), which then remained high for the duration of the experiment. As a result of the increased yield, the CO concentration steadily increased throughout the nonflaming combustion period.

Other patterns of CO evolution from Douglas fir were evident during the various experiments. At 21 percent O_2, the CO yield was nearly zero for the entire duration of flaming combustion. At the transition from flaming to nonflaming (approximately 19 min. into the test), the yield of CO increased over 200 times. In an experiment at an oxygen concentration of 14 percent, the periods of flaming and nonflaming were interspersed. The pattern of very low CO yield during periods of flaming and substantially higher yield during nonflaming was consistent for the alternating periods.

The CO yield for Douglas fir during nonflaming combustion ranged from approximately 30 to 240 times that for flaming combustion, under similar oxygen conditions. For rigid polyurethane foam, the increase in CO yield for nonflaming over flaming was approximately a factor of 20. For PVC, the two tests conducted under nonflaming conditions evolved less CO than the tests which involved flaming combustion.

Within a single mode of burning, the oxygen level was not a significant factor on CO evolution for rigid polyurethane foam or for polyvinyl chloride. However, the evolution of CO from Douglas fir had a greater dependence on oxygen concentration (e.g., the CO yield during flaming combustion increased by a factor of five from 21 percent O_2 to 16 percent O_2). The amount of CO produced by these specimens was independent of the specimen size within the range of 26 to 52 cm^2 surface area.

Oxygen concentration did not affect, in any predictable way, the evolution of HCN or HCl in the experiments conducted in this program.

Conclusions. The conclusions that have been reached thus far regarding oxygen levels in this combustion apparatus are as follows:

1) A change in oxygen level during combustion experiments in the radiant apparatus had a small effect on CO production within a single mode of burning.

2) Mixed modes of combustion (i.e., flaming vs. nonflaming) significantly affected the results of comparative smoke toxicity tests for some materials and care must therefore be exercised in the control of specimen size, in the analysis and control of oxygen concentration, and in the interpretation of the results from such tests.

3) Wood, often considered to be the "standard" for smoke toxicity tests, is a poor choice as such because of the dependence of CO evolution on oxygen concentration.

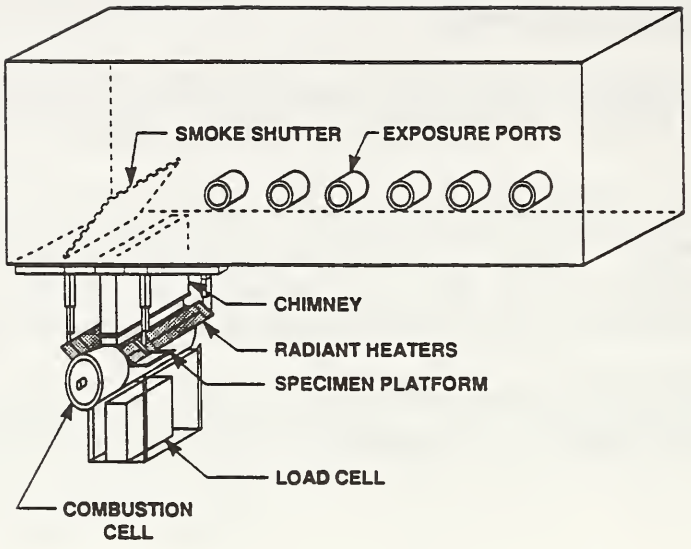


Figure 1. Overall view of the radiant combustion apparatus.

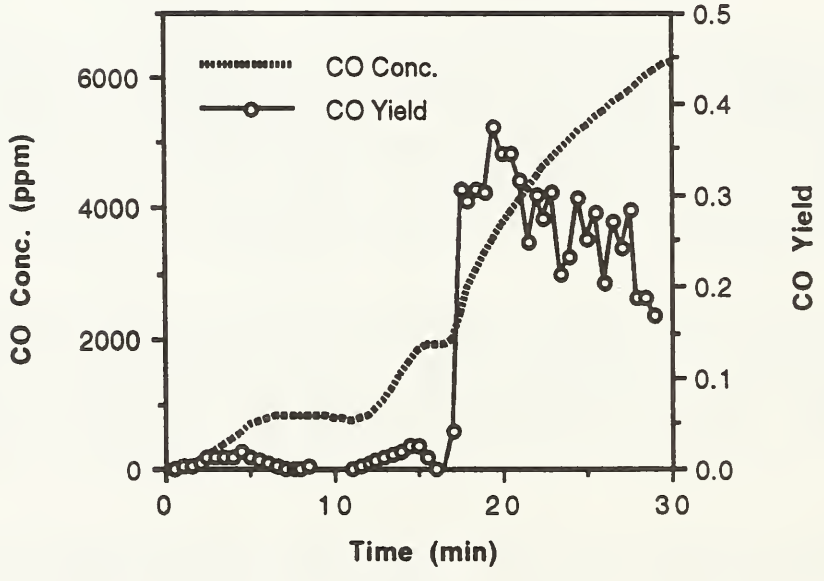


Figure 2. CO concentration and CO yield from Douglas fir at 16 percent O_2.

1.6 Furniture Flammability

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - 1991

FURNITURE FLAMMABILITY

Professional Personnel

H.E. Mitler, Project Leader
T. Ohlemiller, Chemical Engineer
K-M. Tu, Mechanical Engineer
E. Braun, Physicist
T. Cleary, Chemical Engineer

Project Objective

To develop experimental and theoretical methods for predicting the hazard due to the burning of furniture, especially upholstered furniture, when it is ignited.

Scope

Furniture constitutes a major part of the fuel load in residential and commercial occupancies, and therefore we must be able to assess its flammability. An understanding of the way furniture performs when subjected to various ignition sources, and its subsequent burning behavior, will enable manufacturers, standards organizations, and/or regulators to assess the hazard due to that furniture in various occupancies.

Technical Accomplishments

1. Hazard determination.
Three residential scenarios were chosen, as well as a number of actual as well as hypothetical rate of heat release curves from upholstered furniture. HAZARD 1 was run for each of these cases (about two dozen runs in all). It was clear that hazard was serious only when flashover/total room involvement occurred. The program shows that there are circumstances when the house occupants are alerted by a smoke detector, and are thus able to escape, even when flashover occurs. However, recent analyses have shown that only 19% of households have smoke detectors which are actually functioning! Moreover, even in the cases where the house occupants are able to escape, there clearly is considerable risk to the firefighters, after flashsover.

Flashover having been determined to be the critical hazardous event, a criterion for flashover was chosen, and additional runs made, with different RHR curves, to see whether the **shape** of the curve influences a) hazard, and b) whether flashover will occur. The tentative answer is that the shape does matter, so that use of the peak value of the RHR does not always suffice to determine whether flashover will occur. That is, it is more difficult to ascertain, without running a fire model, whether flashover will occur under transient conditions.

2. Ignition modes.
More than three-fourths of residential furniture ignitions are caused by cigarettes, matches, and lighters; the remainder is due to a wide variety of sources, which vary strongly in heat flux, exposure

area, and duration. The question is whether these varied ignition sources result in significantly varying degrees of hazard from a given furniture item.

About 40 chair-burns were carried out. The BFRL furniture calorimeter was calibrated, up to 750 kW output; it appears that it has been reading about 20% low. About 30 runs have been made with Hazard 1, in the standard 6-room "ranch-house" configuration.

The tentative conclusion from preliminary analysis is that the mode of ignition, so long as it is a flaming source, does not matter much in terms of the subsequent fire behavior: the peak height of the RHR curve is about the same in each case, and the time from initial "fire insult" to the peak varies by only a minute or two, for the different igniters. Moreover, it is not clear that the time interval between detection and the peak, varies by even as much as that. From the point of view of safety analysis, the conservative choice is to assume the worst case, in any event.

3. Ignition location.
A similar set of tests was made where the **location** of the ignition was varied. A 10-kW igniter was developed to give a realistic but localized heat source. Twelve chairs were ignited with this source, at different places on the chair(s): on the seat, at the side, at the back, and in front; the chairs were burned in the furniture calorimeter. The results were qualitatively similar to those found in Task 2: for any one model (type) of chair, the resulting RHR curves were very similar, the principal difference being when the peak occurred. The differences among these times, however, were an order of magnitude larger than for the "ignition mode" tests: the largest difference in the location of the peaks was about 30 min. In that case, it is possible that a working smoke detector would have alerted the occupants. To be conservative, however, we must always assume the worst-case scenario, and therefore the differences among the curves is of no significance, in general (although if there is a significant statistical distribution of source locations, the difference implies some fractional improvement in safety).

One significant observation is that an interliner slows the progress of the fire considerably. In Task 2, the related observation was made that when the PU padding is encased in a thin cotton layer, that significantly reduces the ignition propensity and the likelihood of ignition of the PU itself.

4. Furniture model
There would be considerable advantage if one could predict how a furniture item will burn, from just one or two bench-scale tests. This requires a furniture fire model. M. Dietenberger has developed just such a model, but there is some question as to its adequacy. Therefore the last task of this project was to assess the model.

An independent assessment of the Dietenberger furniture-burning model has been obtained, which examined the physics included in the model, the documentation, the validation, and the data input requirements for it. The conclusion is that the model needs improvement in each of these categories. E. Braun is testing the model itself. This phaase of the work is now being completed.

Reports and Publications

"Technical Review of the Furniture Fire Model Version 3," C.L. Beyler.
Four other reports are in preparation.

Related Grants
None

1.7 Wall Fires

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - 1991

WALL FIRE SPREAD

Professional Personnel

H.E. Mitler, Project Leader
K.D. Steckler, Physicist
K-M. Tu, Mech. Engineer
D. Lowe, Technician
W. Rinkinen, Technician
M. McClain, Programmer

Project Objective

To develop a method for predicting the rate and extent of fire spread on interior surfaces in a room using the fire properties of the materials involved. A general model including char-forming materials and composites burning in different configurations including flat walls, corners and ceilings will be completed and experimentally verified by the end of FY 92.

Scope

This project addresses the problem of fire growth on walls in enclosures, the kind of fire which most rapidly leads to flashover. The upward growth rate, especially in a corner, may be thought of as characteristic of the flammability of the burning wall material. Several aspects of wall fire growth will be considered, including growth on flat walls and corners. The burning materials will be arbitrary: from simple, uniform, isotropic, subliming solids to heterogenous, nonisotropic, charring, melting, laminated, and composite materials. Lateral (creeping) spread will also be covered, as well as spread under a variety of external conditions, including burning in a hot, oxygen-vitiated atmosphere.

Technical Accomplishments

The computer program SPREAD, which was developed in FY 89 and 90, calculates the burning rate and upward spread rate of fires on flat walls. This is done numerically, rather than analytically. In FY 91, it has been generalized to include the simultaneous lateral spread of the burning zone. This is calculated using the expression

$$v_s = \Phi/[k\rho c(T_{ig} - T_s)^2] \qquad (1)$$

for the lateral spread rate, where T_s is the instantaneous wall temperature. In a two-zone room fire model, therefore, the spread rate in the upper region will generally be greater than in the lower region. There is a small logistical problem which arises from the fact that the layer height changes with time. This is handled by making small adjustments to v_s such that the instantaneous total pyrolyzing area remains invariant with layer height.

Once ignition has occurred at a node, the surface must regress, as it loses mass. The regression rate is $\dot{m}''/\rho$; we note that it is only necessary to consider the incremental mass losses $\Delta m''(t_s)$, rather than the actual thicknesses. Then burnthrough will have occurred at a node when $\Sigma\Delta m'' \geq m_o''$. When a section burns through, the pyrolyzing area decreases (or increases more slowly), so that the power output goes down, the flame height is smaller, and the spread rate decreases from what it would have been had the section not burned out.

The program has been modified for insertion into CFAST, to the extent possible. The program was delivered to the Hazard Analysis Group in June '91, with extensive documentation. The latter is to be slightly modified, to a NISTIR.

The model has been validated against full-scale experiments carried out by Ken Steckler on PMMA and on wood, and is reported in the documentation mentioned above. Further validation against experiments is now being carried out by Yuji Hasemi, at the BRI.

A method was devised last year, to calculate the pyrolysis rate of an arbitrary material subjected to an arbitrary heating-flux history. The method depends on measuring the heat of gasification as a function of time. If a sample of material is exposed to a heating flux (say, in the Cone Calorimeter), then we define its heat of gasification as

$$h_g \equiv \phi_{net}/\dot{m}'' \tag{2}$$

where $$\phi_{net} \equiv \phi_{in} - \phi_{rr} \tag{3}$$

that is, the incoming flux minus the reradiated flux. Evidently this can (and generally does) vary with time. However, it was expected that (within limits) the heat of gasification will be only weakly dependent on the impinging flux, and will be characteristic of the material. This was found to be the case, this year. In order to calculate the numerator in Eq.(2), the reradiated flux must be found. That is done by measuring the surface temperature of the pyrolyzing material during burning, by using an optical pyrometer. Thus measurements of mass loss rate are made with some prescribed external flux, yielding $h_g(\Delta m'')$ through Eq.(2); then the mass-loss rate for any <u>other</u> flux history will be given, as a function of time, by

$$\dot{m}''(t) = \phi_{net}(t)/h_g(\Delta m'') \tag{4}$$

where $\Delta m''$ is the total mass lost by time t. The method has been validated, and a preliminary report prepared. This method automatically takes transient effects into account, including charring, melting, intumescing, etc.

Theoretical work on the main effects of combustion taking place in a hot, oxygen-vitiated atmosphere has been completed, including the effect on pyrolysis rate. Algorithms have been developed for finding the LOI, the flame temperature, the flame emissivity, and the resulting heating fluxes to the wall. An article on vitiated burning is being prepared; it should be finished by 9/30. This theoretical work has to be validated; to this end, construction was started on an apparatus with which to carry out experiments. Apparatus construction is 95% complete.

One of the input parameters needed to run the model is χ_R, the fraction of the power produced which is radiated away. There is no standard method to do this; however, FMRC has succeeded in developing an apparatus to make this measurement, and this will be used.

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Reports and Publications

"Time-dependent local mass loss rate of finite-thickness burning walls," A.K. Kulkarni, C.I. Kim, and H.E. Mitler, accepted for presentation at the December 1991 ASME Heat Transfer Conference in Atlanta, GA.

"Mathematical Modeling of Enclosure Fires," H.E. Mitler, H.E., Chapter 23 in "Numerical Approaches to Combustion Modeling," (E.S. Oran and J.P. Boris, eds.) Vol.135 of Progress in Astronautics and Aeronautics, published by AIAA, Wahington, D.C., 1991. Also published as NISTIR 90-4294.

Related Grants

"Prediction of Fire Dynamics," R. Alpert and J. deRis, Factory Mutual Research Corp.

"Upward Flame Spread on a Vertical Wall," A. Kulkarni, Pennsylvania State University.

"A Study of Fire-Induced Flow Along the Vertical Corner Wall," K. Saito,
University of Kentucky.

BUILDING AND FIRE RESEARCH LABORATORY
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 91

Institution: Factory Mutual Research Corporation

Grant No.: 60NANB8D0845

Grant Title: Prediction of Fire Dynamics

Principal Investigators: Ronald L. Alpert and John de Ris

Other Professional Personnel: M.A. Delichatsios
H.W. Emmons
G.H. Markstein
L. Orloff

NIST Scientific Officer: Dr. Henri Mitler

Technical Abstract:
This work is divided into four tasks, each of which is designed to provide essential inputs for comprehensive models of burning and fire growth.

Task 1. Prediction of Fire in Buildings (H.W. Emmons)
Progress has been made in the following two areas:
1. Ceiling Jet Dynamics
2. Development of "Strategies for Performance Codes in the U.S."

1. Last year, a top hat theory was presented. Friction and entrainment solutions were both carried to completion. The effect of heat transfer had resulted in a differential equation which had not yet been studied.

Since then an analytical solution has been found which shows that the depth and Richardson number rise as the jet flows along an open ended corridor. As described in detail in "Home Fire Report #82" (and a paper to be presented at the 3rd International Symposium on Fire Safety Science) the top hat steady ceiling jet cannot satisfy the requirement that Ri=1 at the open end.

If friction is present, the appropriate boundary condition can be met only if friction dominates the flow which it generally does not do. There have been no experiments adequately performed to shed light on this problem. However, it is clear that the 1D top hat theory is not adequate. In particular, even the simplest case of no friction, no entrainment and no heat transfer, in which the ceiling jet enters the corridor with an arbitrary depth and surface slope, cannot be described by the simple theory.

2. The paper on Strategies for Performance Codes in the U.S." was the last general presentation at the three-day Conference on Firesafety Design in the 21st Century run by Worcester Polytechnic Institute and SFPE at WPI. The talk assumed that in the next century architects would always design their buildings by CAD methods and that a routine part would be the starting of several fires in different places to check the design's fire safety.

Fire safety means four things; (the specific numbers need to be consensus chosen)
1. All occupants have a 97% chance to escape.

2. No collapse occurs for 20 minutes. (This assumes appropriate fire department action and is designed to protect firefighters.)
3. The total building damage is limited to 25% of initial value.
4. The fire does not spread to adjacent buildings.

The architect would be expected to try several fire protection designs (sprinkler systems, for example) so as to pick the least expensive.

To reach the above capability requires concern for the building contents, windows, and air supply.

To make a fire model of sufficient precision for the above purpose requires an engineering group effort with a detailed report "proving" the validity of each algorithm used. To validate a model, i.e., to compare its prediction with worldwide, first rate fire data, cannot be done casually nor by code officials, but will require a special validation group. Finally, the performance code must be based upon the highest precision available fire model and an extensive study of the socially acceptable risk cost. The paper presents 6 possible approaches of which only one is both practical and acceptable. This approach specifies a probable room fire based upon category of use with an approved and validated model; the building owner-user would be expected to voluntarily keep contents at or below the performance code limit.

Most of the above thoughts are given in more detail in "Home Fire Project Technical Report #83" and will be slightly extended in a report being prepared for publication.

Task 2. Models for Turbulent Flame Chemistry and Radiation (J. de Ris, L. Orloff)

Perhaps the two most urgent and challenging problems of fire research are the prediction of fire burning (heat release) rates and the release of toxic (or otherwise damaging) products of incomplete combustion. The heat release rates for hazardous-scale fires are generally governed by the radiant heat feedback to the pyrolyzing surface from the flames. Over the past several years we have established that the radiant fraction of the heat release rate is governed by the fuel smoke point which provides a convenient measure of flame sootiness. Radiant fractions have now been measured and correlated for a wide range of hydrocarbon fuels, fuel mixtures, fuel dilutions with nitrogen and ambient oxygen concentrations. The correlations of turbulent radiant fractions against the laminar flame smoke points are considerably improved when the comparisons are made at fixed adiabatic stoichiometric flame temperatures and oxidant to fuel stoichiometric ratios. This work should be appearing in the published literature shortly[8].

The understanding of flame radiation from our many studies have resulted in the development of a Global Flame Radiation Model which predicts the overall flame radiant fraction in terms of the fuel smoke point and incompleteness of combustion and is in excellent agreement with experiment. The model provides the radiation from both the luminous soot and the non-luminous gaseous products of combustion either of which can be dominant, depending on the fuel smoke point (i.e. flame sootiness). By assuming the soot formation is proportional to the overall fluid flow time (rather than the Kolmogorov microscale time), the model predicts the experimentally observed increase in radiant fraction with overall heat rate for axisymmetric and planar flames. This

assumption is consistent with the view of soot formation occurring principally in the bulk hot flow rather than only along thin flame sheets. It is also supported by Kent's[1] correlation of soot concentration and temperature profiles at fixed overall flow times.

At present the above Global Model has been tested only against fuels burning in air, because it needs to be supplied with incompleteness of combustion data which are not generally available for other ambients. To fully establish this radiation model, or indeed any combustion model, it is important for it to be tested in more general ambient atmospheres. Hence this project is currently measuring the incompleteness of combustion over the same broad range of fuel/ambient conditions for which we already have radiant fraction measurements.

At this time we have largely mastered the problem of predicting the overall radiant fraction from simple buoyant turbulent diffusion flames by performing extensive experimental measurements, finding correlations of this data and now more recently developing the Global model. Our efforts are now devoted toward understanding the thermo-chemistry in flames which controls the: incompleteness of combustion, release of toxic products of combustion, and most importantly the vertical distribution of radiation which governs upward fire spread and steady burning rates. These issues cannot be resolved by a global model which treats the flame as a whole.

The attached schematic summarizes our proposed model for buoyant turbulent diffusion flame combustion. The model is tailored specifically for fire research applications requiring predictions of: 1) flame radiation versus height and fuel type, needed for models of upward fire spread and steady burning, and 2) the release rates of soot, CO and other toxic or damaging products of incomplete combustion. Because the processes of flame radiation and flame chemistry are so tightly coupled in nature they must be modeled together. Flame radiation is controlled by the thermo-chemistry of soot formation and oxidation; whereas flame chemistry and temperature are governed by the radiant cooling of the flames resulting in their radiant extinction and release of products of incomplete combustion. The proposed model is applicable to general hydrocarbon/O_2/N_2 oxidant turbulent diffusion flames. It is supplied with an "exact" multi-step chemical kinetic reaction mechanism for the oxidation of soot, CO, H_2, etc. For future applications the reaction mechanism can be readily augmented to examine the effects of chemical additives, such as halogens (Br, Cℓ, I, etc.) whose combustion kinetics are known. The model predicts the soot formation rate for each hydrocarbon fuel/oxidant combination in terms of its corresponding laminar flame smoke-point flame height, ℓ_s.

The proposed turbulent flame chemistry and radiation model employs a probability density function (Pdf) to describe the effects of turbulence on the species concentrations. The Pdf for a passive scalar is explicitly calculated by a so-called "coalescence/dispersion" or "stochastic mixing" model[2] for the turbulence fluctuations. Such models can be coupled in a physically meaningful way with standard chemical kinetic models to calculate species concentrations. However, present coalescence/dispersion models which are based on differential equations do not correctly treat the effects of turbulence leading to improper (non-Gaussian) decay of scalar fluctuations in a homogeneous turbulent flow. This problem can be overcome by calculating Pdf's with relatively simple integral equations which model the turbulent cascade process and

Turbulent Diffusion Flame Combustion Model for Flame Chemistry and Radiation

Physico-Chemical Processes

Implementation

Turbulent (Buoyant) Fluid Dynamics

↓

Turbulent Mixing - Conserved Scalar P*df*

↓

Mixing Driven (Rapid) Chemistry

Fuel + Oxidant $\longrightarrow$ CO, H_2, CO_2, H_2O
Fuel consumed by diffusion controlled, highly localized combustion driven by the turbulent scalar dissipation.

↓

Bulk (Slow) Chemistry & Radiation

1. CO, H_2 oxidation kinetics
2. Soot Formation: $D(\rho Y_S)/Dt=(\rho Y_F A_s/l_s)e^{-Es/RT}$
3. Soot Oxidation: $C_s + OH \rightarrow CO + H$
4. Radiation: $D(\rho H)/Dt=-\dot{q}'''_R=-(\dot{q}'''_{Rs} + \dot{q}'''_{Rg})$

Density

κ-ε, or Morton-Taylor Entrainment Model

"g" of κ-ε-g, or Stochastic Mixing Model

From Sivathanu-Faeth empirical correlation of major species versus mixture fraction in hydrocarbon/air laminar diffusion flames.

CHEMKIN - Extensions

1. Warnatz reduced mechanism
2. From hydrocarbon smoke-point
3. Neoh mechanism with fixed particle size
4. From Modak and/or Grosshandler

can be adjusted to yield the experimentally observed Gaussian decay for homogeneous turbulent flows.

The key concept introduced by the model entails the splitting of the rapid turbulent mixing processes (controlling the hydrocarbon fuel consumption) from the considerably slower bulk flow processes (soot formation, soot (and CO) oxidation and radiant heat loss). These two sets of processes are treated separately. Rapid turbulent mixing results in highly localized moving flame sheets which consume the supplied oxidant and hydrocarbon fuel while producing principally CO, H_2, CO_2 and H_2O. Fortunately the local concentrations of the major species are well correlated against the local equivalence ratio (or mixture fraction) independent of the local straining (mixing) rate; so that one can employ Sivathanu and Faeth's[3] correlation of concentrations for general hydrocarbon/air laminar flames to infer the fuel consumption rate in terms of the evolving scalar Pdf. We note here that the mixing rates for the rather lazy flames characteristic of fires almost always result in micro-scale flow times (3-20 ms) that are considerably larger than the characteristic chemical times (< 3 ms) for significant heat release; so we need not consider local flame extinction, turbulent lift-off or other extinction phenomena due to rapid mixing.

The much slower (20-500 ms) processes of soot formation, soot[5] (and CO) oxidation and flame radiation are modeled by suitable extensions[4] of the CHEMKIN code which calculates the evolution of the composition and temperature for a well-mixed plug-flow reacting gas. Separate CHEMKIN calculations are made for each mixture fraction at each flame elevation. Effects of inter-eddy-mixing at each elevation are included through a partial interchange of fluid elements of different mixture fractions consistent with the stochastic Pdf model formulation. Conventional Pdf models for turbulent diffusion flames ascribe a particular chemical composition and temperature to each value of the mixture fraction scalar. The present model relaxes this constraint and allows chemical reactions and radiant emission to proceed for each Pdf mixture fraction as it evolves with the flow. The model specifies an ensemble of temperatures, soot volume fractions, and gaseous concentrations at each elevation consistent with actual turbulent diffusion flames. The non-isothermal model of Modak and Grosshandler[6,7] can explicitly calculate the radiation for such situations.

The overall 1-D model described here has only five "adjustable" constants: 1) entrainment constant; 2) mixing constant, 3) pre-exponential soot formation constant, A_s, 4) soot formation activation energy, E_s, and 5) soot particle size, d_s. Most of these constants are not really adjustable in view of the numerous constraints imposed by available experimental data. We will focus on correlations of data for incompleteness of combustion in various ambients and the vertical distribution of radiant emission for fixing these constants; so that the model can be used more immediately for fire research applications.

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Task 3. Models for Wall Fire Flame Radiation (G.H. Markstein)

Theoretical models of wall burning and vertical fire spread have been developed at FMRC and elsewhere. However, all these models lack a predictive input for flame radiation which controls the burning process. Development of useful predictive submodels of wall flame heat transfer for inclusion in comprehensive fire growth models is the ultimate objective of this work.

Under the present task, measurements are currently performed on gaseous-fuel wall flames generated by water-cooled vertical sintered-metal burners. The fuel mass transfer rate is set by electronic mass-flow controllers. The instrumentation includes: 1) a wide-view-angle radiometer measuring total radiant emission; 2) a slit scanning radiometer to determine the vertical distribution of radiant emission by horizontal slices across the wall fire; and 3) differential thermocouples for measuring the total heat transfer back to the wall; 4) a new dual radiometric instrument, now being constructed, for measuring the optical thickness of the flames. The use of other instrumentation to measure geometrical flame thickness, soot volume fraction, and radiation temperature is being considered.

The burner consists of ten 132 mm high and 380 mm wide porous-metal panels topped by a 660 mm high water-cooled heat transfer plate. It is provided with water-cooled sidewalls and with water-cooling passages embedded in the porous metal and instrumented with differential thermocouples for measurement of total heat transfer. The heat-transfer distribution to the metal plate above the burner is also measured by differential thermocouples.

An essential part of the instrumentation for the wall-fire study is a scanning radiometer that measures the vertical distribution of radiant emission per unit height of horizontal slices across the fire. The signal-to-noise ratio and the linearity of angular deflection of the instrument currently used have been greatly improved with respect to those of an earlier version by the use of spherical-mirror optics and of feed-back-controlled driver circuit for the scanning galvanometer.

The current phase of this task deals with vertical distributions of flame heat transfer within the gas-supply (or "pyrolysis") zone. In particular, pyrolysis zone correlations for a set of recent data obtained with propylene supplied to six burner panels are shown in Figures 1 to 4. Here, $\dot{q}''_r$ is the radiant power per unit flame area, derived from the scanning-radiometer data under the assumption of isotropic emission by optically thin flames, and $\dot{m}''$ is the fuel mass flux. Figure 1 shows a transition at a critical mass flux, $\dot{m}''_c$, defining two sharply separated regimes. In each regime, linear relationships

$$\frac{1}{\dot{q}''_r} = \frac{1}{\dot{q}''_\infty} + \frac{s}{\dot{m}''} \qquad (1)$$

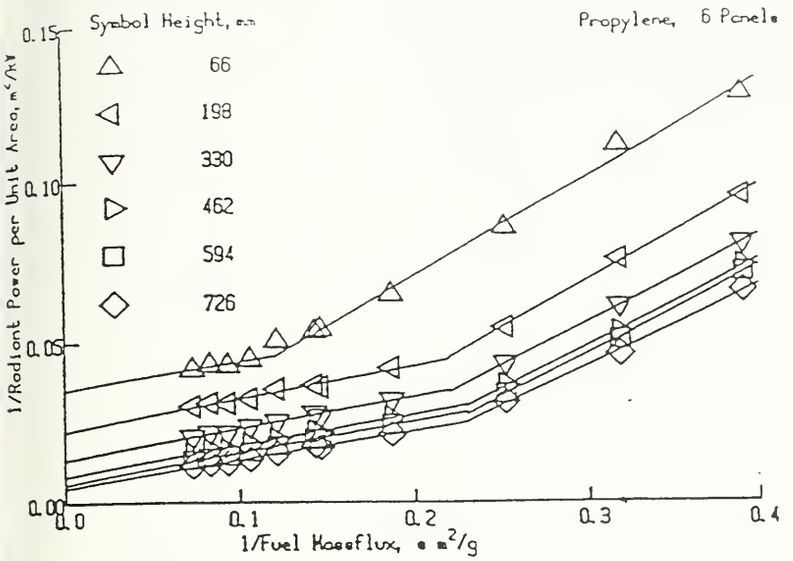

Fig. 1. Plot of $1/\dot{q}''_r$ vs $1/\dot{m}''$ for propylene wall fires of 792 mm simulated pyrolysis height. Here, $\dot{q}''_r$ represents the radiant power emitted by unit flame area under the assumption of isotropic emission by optically thin flames.

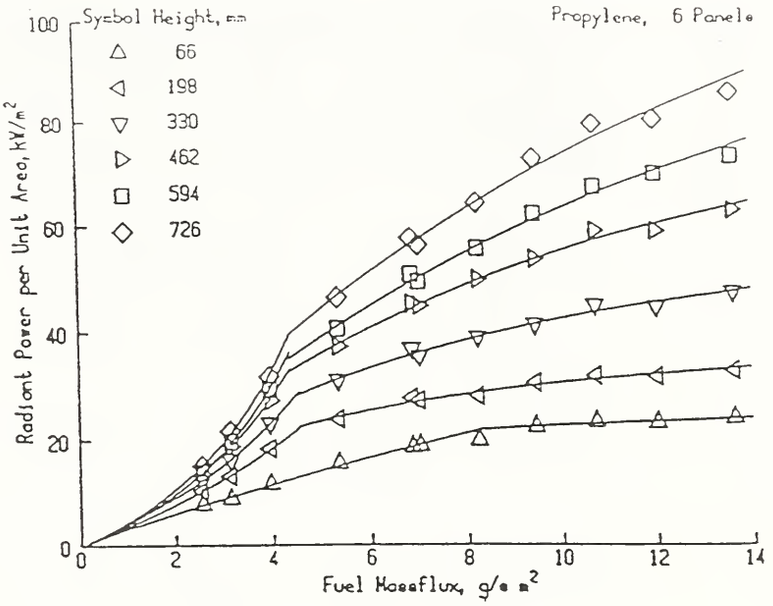

Fig. 2. Plot of $\dot{q}''_r$ vs $\dot{m}''$, data of Fig. 1.

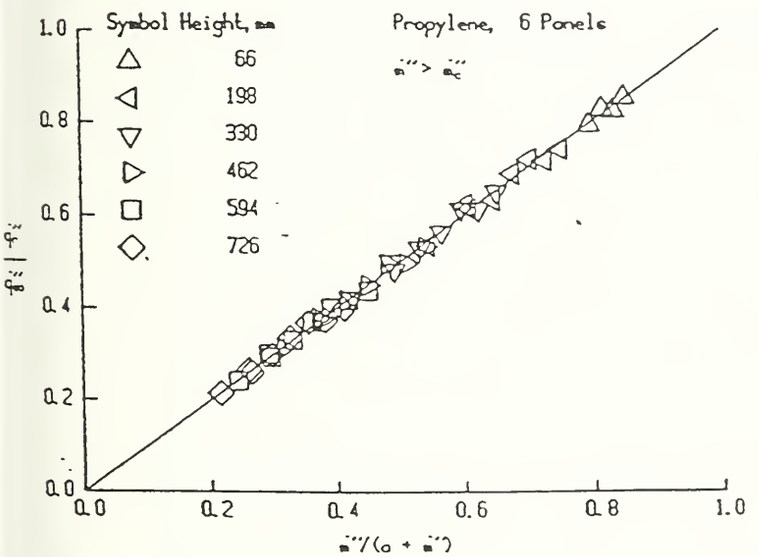

Fig. 3 Dimensionless correlation of the data of Fig. 1 for $\dot{m}'' > \dot{m}''_c$

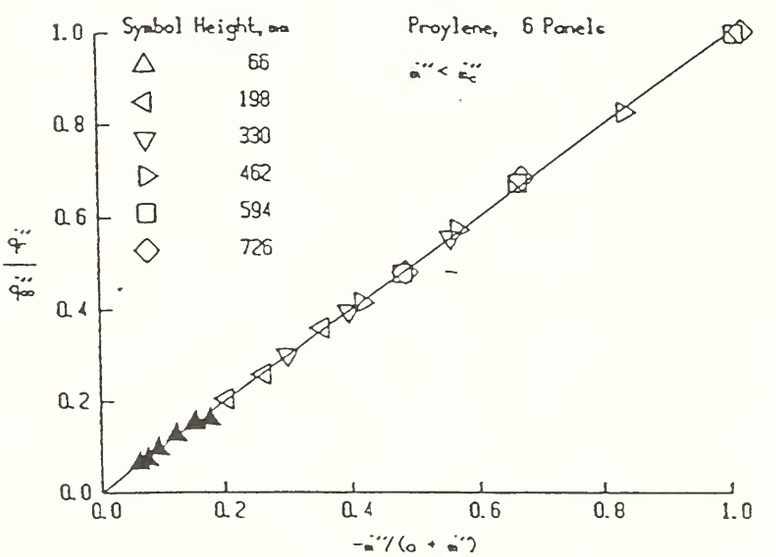

Fig. 4 Dimensionless correlation of the data of Fig. 1 for $\dot{m}'' < \dot{m}''_c$. Solid symbols correspond to positive coordinate values (Z = 66 mm).

are seen to be satisfied for any given height, z, with slopes, s, nearly independent of z. The critical mass flux, $\dot{m}''_c$, is seen to be also nearly independent of z, except for the lowest height of 66 mm. It's value, about 4 g/sm^2, agrees with that of transition from extinction to flaming generally observed for solid-fuel burning[3].

The dimensionless correlations shown in Figs. 3 and 4 were obtained by rewriting eq. (1) in the form:

$$\frac{\dot{q}''_r}{\dot{q}''_\infty} = \frac{\dot{m}''}{\dot{m}'' + a} \quad \text{where } a = \dot{q}''_\infty \, s \tag{2}$$

It is expected that such correlations can be generalized to other fuels and extended ranges of pyrolysis height and fuel mass flux, when additional data will be available.

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Task 4. Transient Pyrolysis, Flame Radiation and Sooting Properties of Solid Materials (M.A. Delichatsios)

A new integral thermal pyrolysis model[4] for the transient pyrolysis of charring and non-charring materials has been developed and evaluated by comparison of the results with exact solutions. The pyrolyzing material is divided into a char layer and a virgin layer where the material has not yet pyrolyzed. These two layers are separated by an isothermal interface which is at a pyrolysis temperature (characteristic of the material). At this interface, heat is transferred to the virgin layer, causing further pyrolysis of the material. A one-dimensional transient heat conduction model is used to predict the heat transfer within the material. Exponential temperature profiles were assumed for the heat conduction model. Using a two-equation θ-moment method, the original partial differential equations were transformed into a set of two ordinary differential equations for each layer. These equations were numerically solved to determine the pyrolysis rate, regression depth and surface temperature. The model has been shown to be very accurate (errors $\leq$ 2%) by comparisons of numerical results with exact solutions. The accuracy of the integral model together with its simplicity has allowed the deduction of pyrolysis properties of materials by using simple flammability test data, as described below.

The methodology developed for deducing material properties both for non-charring and charring material pyrolysis uses measurements in existing flammability apparatus. The methodology has been described in detail in the thesis of Y. Chen[1]. For completeness, we outline this methodology here:

1. Preheating - Before Pyrolysis Starts. The same methodology is used for non-charring and charring materials. The thermal properties of the virgin fuel (k,ρ,C) and an apparent pyrolysis temperature (T_p) are deduced from measurements such as a) surface temperature histories, b) ignition times, c) weight loss histories at various fixed constant heat fluxes. The methodology for obtaining the virgin properties has been explained in detail in a recent publication[2] and report[3].

2. Pyrolysis Rates-Properties. By using the experimental measurements of surface temperature and weight loss histories after pyrolysis starts together with an accurate integral model for pyrolysis[1], we have developed and validated a methodology for obtaining the pyrolysis parameters for 1) non-charring [i.e., ΔH_v heat of gasification = $L + C_p \Delta T_p$, $\frac{L}{C_p \Delta T_p} = \frac{L}{C_p (T_p - T_o)} = \lambda$] and 2) charring fuels [i.e., ΔH_v, λ, and char conductivity k_c]. A significant result from this analysis and comparison with experiments for charring materials[1], is that the pyrolysis process is dominated by the reradiation losses from the surface of the char to the extent that the thermal capacity of the char has a negligible effect on the pyrolysis rate histories. As reported in the previous quarterly report, the methodology was validated for pure cellulosic boards[1]. During this quarter, we have demonstrated and applied the methodology for two different particle boards (the so-called NBS particle board and the FAA particle board), both for thermally thick and thermally intermediate conditions. Figure 1 illustrates the success of the present methodology. The ordinate in the figure is proportional to the mass loss at time, t, normalized by the thermal depth:

$$(1 + \lambda) \frac{x_p}{\delta_v} = \text{ordinate} \tag{1a}$$

where

$$x_p = \frac{\dot{m}''}{\rho_v - \rho_c} \tag{1b}$$

$$\delta_v = \frac{k_v (T_p - T_o)}{\dot{q}_o'' - \sigma T_p^4} \tag{1c}$$

$$\lambda = \frac{L}{C_p (T_p - T_o)} \tag{1d}$$

ρ_v = virgin density, ρ_c = char density.

The abscissa in Figure 1 is the time from the beginning of pyrolysis ($t - t_p$) normalized by a characteristic pyrolyzing time $\frac{(k\rho C)_v (T_p - T_o)^2}{(\dot{q}_o - \sigma T_p^4)^2}$.

The virgin properties of the particle board shown on the figure were obtained from the preheating tests[2,3] (this methodology will be summarized in the annual report). The values of $\lambda = 0$ and $k_c = .2248$ W/mK (char conductivity) were obtained by comparison of the model predictions with experimental data

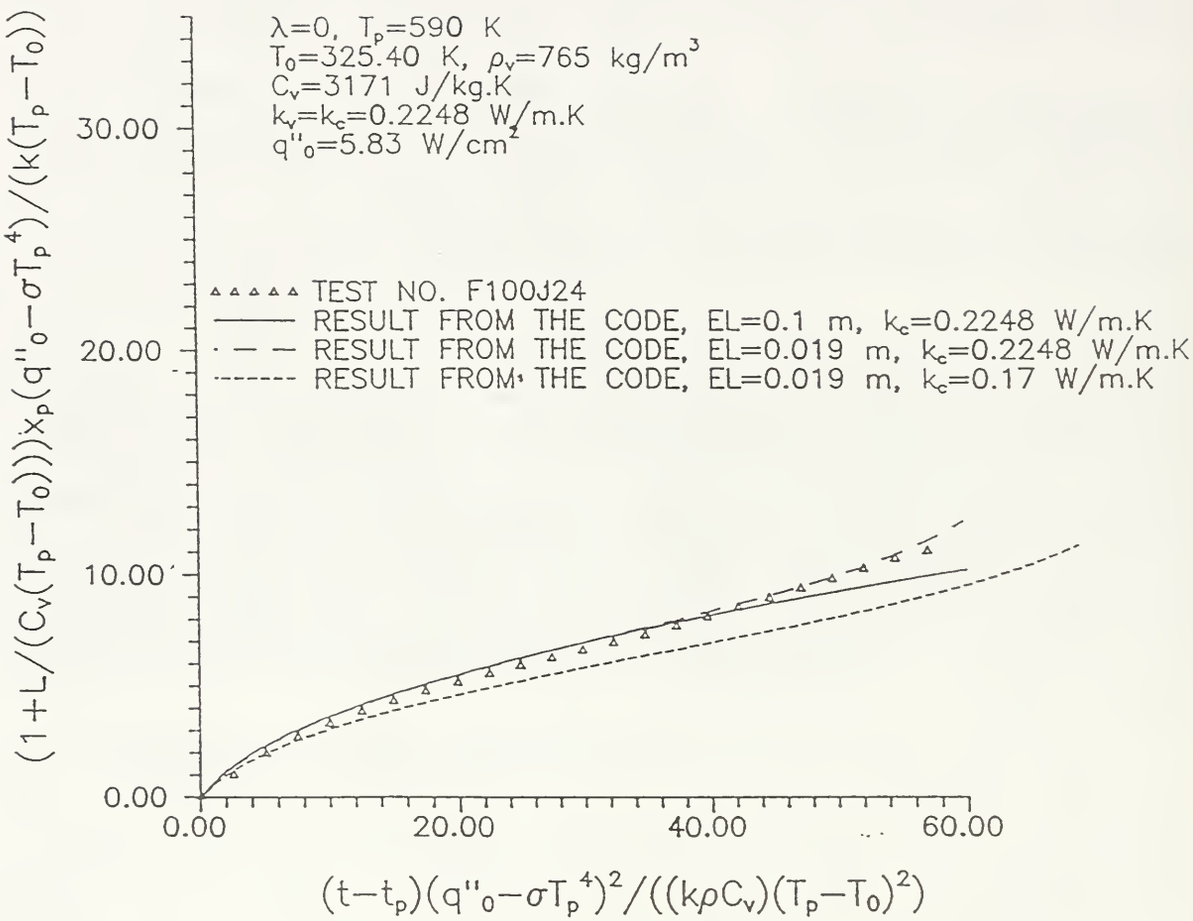

Figure 1. An illustration of the methodology for obtaining material properties for predicting mass pyrolysis histories. Here the mass loss (~ X_p = pyrolysis depth) normalized by the thermal length is plotted vs the time normalized by a characteristic pyrolysis time (EL is the material thickness for the particle board test data EL = 1.9 cm).

for an imposed heat flux at $\dot{q}''_o$ = 3.55 W/cm^2. Then, these values were used to predict the mass loss for other imposed heat fluxes such as the one shown in Figure 1, $\dot{q}''_o$ = 5.83 W/cm^2. For comparison, we have plotted in this figure, together with the experimental data, three model predictions.

1) for infinitely thermally thick solid, δ = 10 cm, k_c = .2248 W/m K.

2) for intermediately thermally thick solid representing the test conditions δ = 1.9 cm, k_c = .2248 W/mk.

3) for intermediately thermally thick solid δ = 1.9 cm, but for k_c = .17W/mk.

The ability of the model, which uses predicted char properties, to predict mass loss histories (case 2 above) seems to be more than adequate for applying this methodology to fire hazard and fire growth predictions.

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BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 91

Institution: The University of Kentucky

Grant No.: 60NANB1D1142

Grant Title: A Study of Fire Induced Flow along the Vertical Corner Wall: Part II

Principal Investigator: Kozo Saito
Associate Professor
Dept. of Mechanical Engineering

Co-Principal Investigators: W.A. Gruver
Director
Center for Robotics and Manufacturing Systems

S.N. Singh
Professor
Dept. of Mechanical Engineering

Other Professional Personnel: Cheng Quin, Doctoral Student
Wen Lin, Master Student
Akira Arakawa, Visiting Scientist
Toshi Daikoku, Visiting Scientist
Akihiko Ito, Visiting Scientist

NIST Scientific Officer: Dr. Henry Mitler

TECHNICAL ABSTRACT:

This research is a continuation of the previous project. We are conducting this research project based on our philosophy: "Observation comes first, then modeling", in other words,"Careful experiments are the source of creativity (modeling)". Previously, we visualized fire induced flow along the vertical corner wall changing heat flux and burner stand-off distance using methane and propane burners. In that project, we completed the following tasks: (1) Design of a reduced-scale model with Marinite walls, a square shape gas burner (0.15cm x0.15cm x 0.08cm) and a flow visualization system. (2) Visualization of fire induced flow as a function of the burner heat flux (0, 20, 40, 60, 80 and 100 W/cm^2), and the burner stand-off distance (0,0.012, 0.1, 0.15 and 0.20 m). We found that that under some conditions a vortex tube appeared near the burner corner and propagated along the corner to the ceiling. If the vortex tube formation occurred during upward flame spread, it may enhance the

flame spread rate significantly [1,2]. Thus the experimental study to further understand the conditions under which the vortex is formed and its impact on the upward spread rate is investigated in this study. (3) Application of infrared radiometry, IR, for measurement of transient fire heated wall temperatures. Exploratory tests were performed to map the fire heated wall temperature using an IR system with automated image analysis for a typical heat flux and burner stand-off distance. A difficulty encountered while using the IR camera system which is located away from the fire source, is that it must measure the wall temperature through the flame. Thus, we were able to characterize the two dimensional behavior of the flame spread from the instantaneous temperature mapping of the wall surface [3]. These data are expected to improve our current knowledge of upward flame spread [4] and help to develop a more accurate prediction model [5,6].

Based on the above progress, we are conducting the following experiments: (1) Effect of burner geometry on fire-induced flow; (2) Effect of the flame characteristics on IR temperature mapping; (3) A series of IR temperature mappings of the fire heated wall and heat flux measurements at the fire heated wall; (4) Flame height measurements of the upward and horizontal flame spread rate along the vertical corner wall; and (plume velocity and entrainment measurements.

In this abstract, we report only the results on topics (1) and (2).

Effect of Burner Geometry on Fire-Induced Flow

In the 1990 project, using a square gas burner, we observed vortex tube formation. It is important to understand the conditions of the vortex formation, and determine whether the observed vortex is peculiar to the square gas burner, and its effects on the spread rate. To do that, we lifted the floor to the same level of the top rim of the gas burner, and then inserted the burner in a square-cut hole. Experiments were performed using a Marinite corner wall (where there is no flame spread). Flow visualization experiments changing the burner heat flux (0, 20, 40, 60, 80, and 100 W/cm^2) and the burner stand-off distance (0, 0.025, 0.10, 0.15 and 0.20 m) confirmed the previous results, and we observed vortices under the same conditions as in the previous experiments. As a next phase we are planning to extend our experiments under the upward flame spread condition.

Effect of Flame Luminosity on the IR Temperature Mapping

Previously, the IR system was successfully applied to obtain wall temperature distributions generated by a premixed methane-air flame. Prior to application of the IR system for realistic situations burning different kinds of fuel, it is necessary to know how accurately the IR system can perform a through-flame measurement for different fuels. To do this, first we used propane as a fire source and repeated the same temperature mapping experiments as previously; then, the results were compared to the thermocouple based results. Secondly, we conducted exploratory upward flame spread tests using a corner

wall made of cardboard with dimmensions 0.5 mm in thickness, 0.30m in width, 1.0m in length. To check the difference of emissivity and the effect of char on the IR measurement system, we conducted one experiment using black cardboard, and another experiment using white cardboard. Furthermore, we conducted an upward flame spread test on a flat wall made of black cardboard for comparison. Spread behavior was recorded using the IR system and results were obtained every 10s after ignition of the burner (which was placed at the bottom of the sample). The mapped wall temperature distribution was color coded and shown in Fig. 1. As a result, we found that the IR system using a 10.6 micron filter can detect wall temperature distributions for methane, propane, and black/white paper.

As a next phase of this project, we are in the process to conduct experiments on the other topics mentioned earlier.

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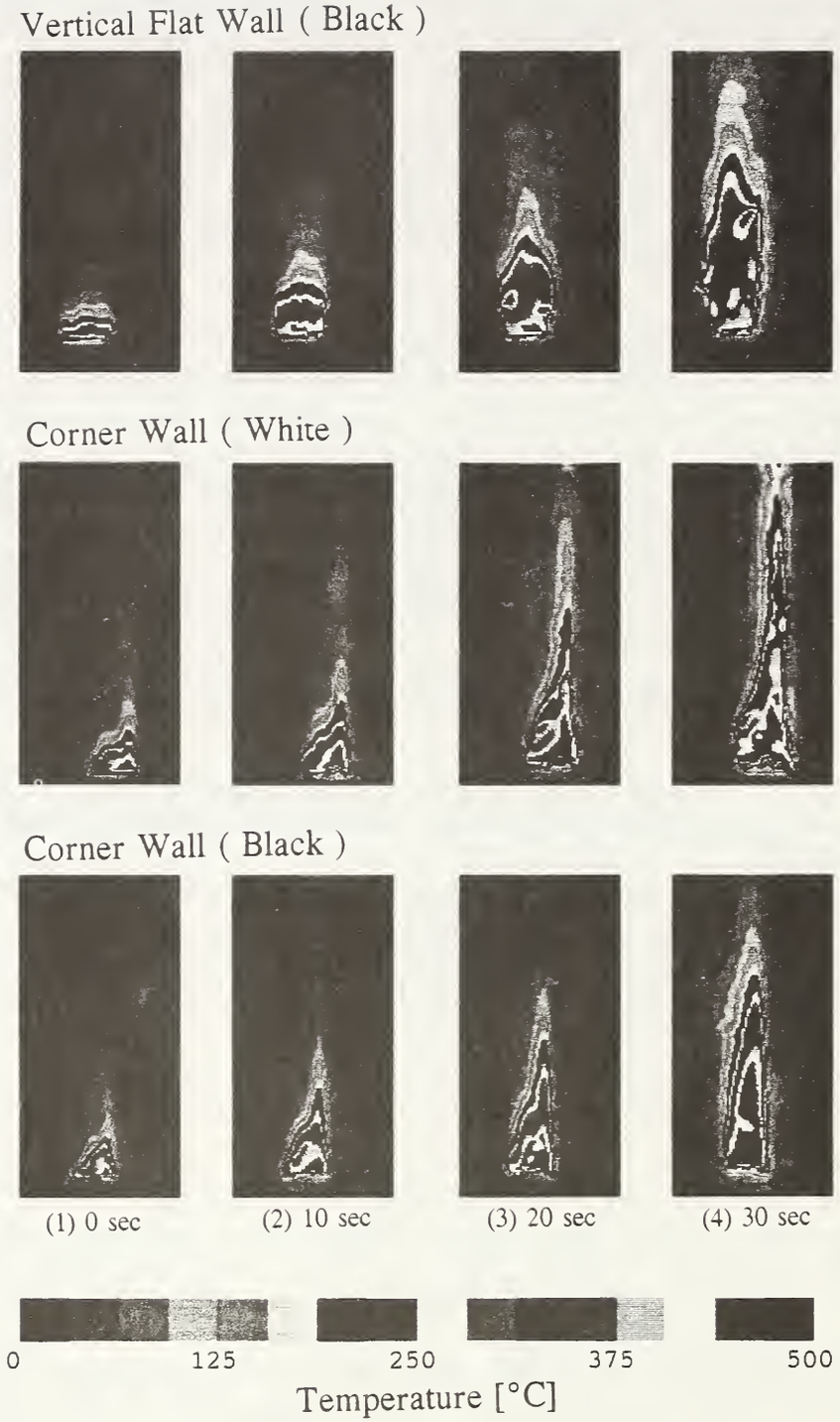

Figure 1 Temperature profiles of vertical flat and corner walls obtained by IR system with a 10.6 micron filter. The walls were ingited at the bottom and flame is spreading upward.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution:	The Pennsylvania State University
Grant No:	60 NANB8D0849
Grant Title:	Upward Flame Spread on a Vertical Wall Under External Radiation
Principal Investigator:	Professor Anil K. Kulkarni Department of Mechanical Engineering 209 Mechanical Engineering Building The Pennsylvania State University University Park, PA 16802
Other Professional Personnel:	Ellen Brehob, Doctoral Student ChoongIk Kim, Doctoral Student Shailesh Manohar, Graduate Student
NIST Scientific Officer:	Dr. Henri E. Mitler

Technical Abstract:

Introduction: In many enclosure and corridor fires,radiation from the surrounding walls has a significant effect on the spread rate of flames on walls that are yet to burn. The overall objective of the project is to study the upward flame spread under external radiation flux similar to that caused by the surrounding fire. When a wall exposed to a high level of external radiation is ignited at the bottom, the upward flame spread characteristics can be significantly affected in three ways: 1) For most materials, the external heat flux can be crucial in sustaining the flame spread for an ignited wall which would otherwise burn itself out. 2) The external radiation heat flux will heat up the yet-unpyrolyzed area of the wall ahead of the pyrolysis front, causing it to reach the pyrolysis temperature sooner, thus enhancing the upward flame spread rate. 3) The external heat flux will enhance the burning rate of the ignited area, causing larger flames and faster upward flame spread. In the present project, which began in August 1990, experimental and theoretical studies are in progress to investigate the problem of upward flame spread under external radiation, and they are divided into three major tasks, as described below.

Upward Flame Spread Experiments: A new flame spread facility has been designed and completed in which wall samples of 0.3 m by 1.2 m (1' x 4') are subjected to radiation heat fluxes of up to 28 kW/m^2 using two large heated radiant panels, each consuming up to 23 kW of electric power from a 440 V, 3-phase, 60 amp power supply (see Figure 1). The two infrared heating panels are angled towards the wall sample and placed 0.3 m away from it. The radiant panels are made of rows of heating elements embedded in a ceramic material with a Corning Vycor face plate, which can be heated to 815 K, encased in a steel enclosure of 0.30 m width and 1.27 m height. In order to control the large current and voltage required for the radiation panels a silicon control rectifier (SCR) is used. Water-cooled side shields are attached to the marinite panel and bent forward at a 45 degree angle to contain the unwanted radiant energy from the heating panels, to minimize cross-flow, and to keep the flames from wrapping around the sample. A 0.4 m long line-burner, supplied with propane, is used to ignite the wall samples. Among the major components of instrumentation are, a Sony Handycam (CDC-F77) video camera recorder with a shutter speed of 25 microseconds to record the flame spread event, circular foil (Gardon) heat flux gauges to

measure the radiant flux and flame heat feedback, and thermocouples mounted in the material sample to measure the surface temperature of the sample.

At present, preliminary experiments on the measurement of uniformity of heat flux distribution and calibration are in progress. Overall, our facility for studying turbulent upward flame spread under external flux simulating a surrounding fire is similar to that of Dr. Yuji Hasemi's facility at the Building Research Institute in Japan. The two facilities, which were conceived and developed independently, are complementary and will allow development and verification of "small" (but turbulent) scale tests.

Local Mass Loss Rate Experiments: In the mathematical model for prediction of upward flame spread rate under external radiation, knowledge of local mass loss (or burning) rate is essential. This property may be either calculated based on certain assumptions, or it can be measured as explained in publication 9. In the the present project, it is measured using an apparatus described in publication 10. A 12 cm x 12 cm piece of sample material is mounted vertically, covered with turbulent flames, and exposed to external radiation, in a configuration similar to that of a wall having upward spreading flames.

The mass of the sample is measured continuously by an electronic balance, and the output voltage from the balance is fed to the data acquisition system. The raw data are smoothed, fitted to a fifth order polynomial approximation, and then the time derivative is calculated. The resulting fourth order polynomial equation represents the mass loss rate function for the sample material under a specific level of external heat flux. Results for Masonite samples at four different levels of radiant flux are shown in Figure 2. As the level of radiant flux was increased, the mass loss rate rose more steeply and then dropped to zero more quickly. This can be related to a more rapid rise in heat release rate, and a shorter burn-out time for the fuel.

Future work will entail mass loss measurements for other materials, in addition to the data for Masonite presented here. The experimentally measured local mass loss rate curves will be used in a numerical model to predict upward flame spread under external radiation.

In-depth Radiation Absorption Experiments: The absorption coefficient (alternatively expressed as the in-depth absorption length) is important in assessing the in-depth radiation absorption effects. In particular, it is an essential input to a mathematical model that attempts to predict upward flame spread subjected to strong external radiation. Plastics such as polymethylmethacrylate (PMMA) can absorb external radiation in-depth to a significant degree, and it depends on the spectral characteristics of incoming radiation during the heat up time. After surface pyrolysis, the transmittance of PMMA samples reduces significantly since the surface is rough, with trapped bubbles, and soot contamination. Very little quantitative information is available on this property for most practical materials. In the current project we have started experiments for the determination of radiative properties of real materials. So far, we have set up the apparatus and then made transmittance measurements for PMMA slabs, before and after surface pyrolysis. The spectral and mean absorption coefficients are computed using a known set of equations; more details on this work are given in publication 11.

In the experiments, the total transmittance is measured over the wavelength range 1 μm to 20 μm. The measurements were carried out using a standard Fourier transform infrared spectrometer (FTIR). The FTIR is capable of handling wavelengths ranging from near to far IR using three different detectors and two beamsplitters. Figure 3 shows the absorption coefficient for unburnt samples. The region from wavenumber 500 to 2000 (expressed in cm^{-1}) and around 3000 shows a number of spikes. It is due to the fact that the transmittance in this region is very low, and hence the FTIR output is not very accurate. The best results were obtained in the region from 4000 to 10000 wavenumber (2.5 μm to 1 μm wavelength).

For practical usefulness of the present measurements, the Planck mean absorption coefficient was calculated for a range of blackbody source temperatures and plotted in Figure 4. Mathematical models predicting rate of heat release or upward flame spread on a burning vertical wall require a mean absorption coefficient as an input to account for the energy absorbed from an external source. Depending upon the estimated equivalent black body temperature of the source, such as burning surrounding walls or hot objects, the mean absorption coefficient can be read off from Figure 4 and used in the models.

After the surface of the PMMA slab is pyrolyzed, there is a marked decrease in the transmittance. The 1/16" and 1/8" thick samples yielded practically zero transmittance up to 4000 wavenumber, and approximately 5% to 10% at a higher wavenumber. The slab can no longer be considered to be homogeneous and the properties of the pyrolyzed surface must be accounted for. The above method of estimating the absorption coefficient does not apply here, therefore, alternative techniques have to be used. Currently, we are building a heated cavity reflectometer for these measurements.

Experimentally measured flame spread data, an appropriately validated model, and radiative properties of materials obtained here should be extremely useful in fire hazard codes for single or multiple enclosures, as well as for assessing material flammability in relevant orientation.

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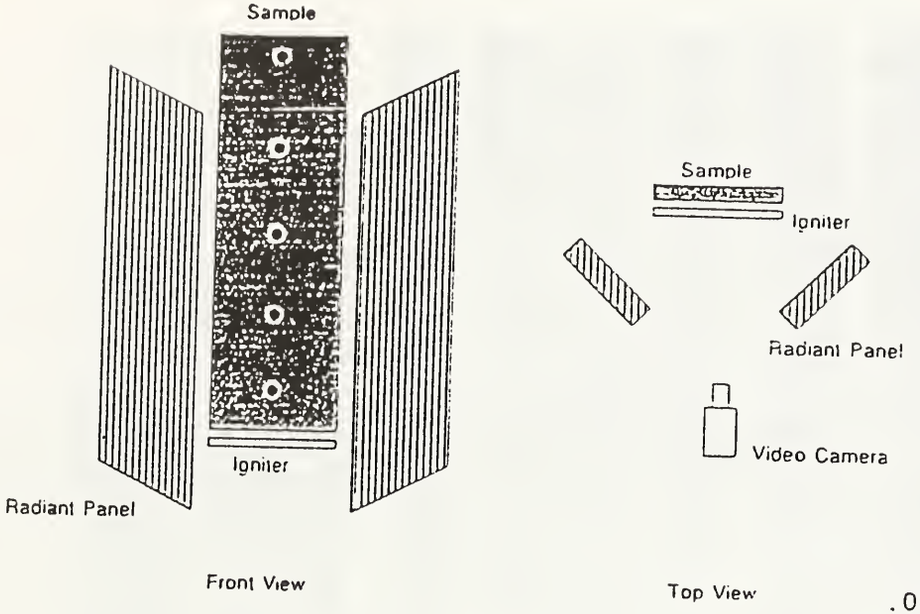


Figure 1. Experimental Setup for Upward Flame Spread Under External Radiation

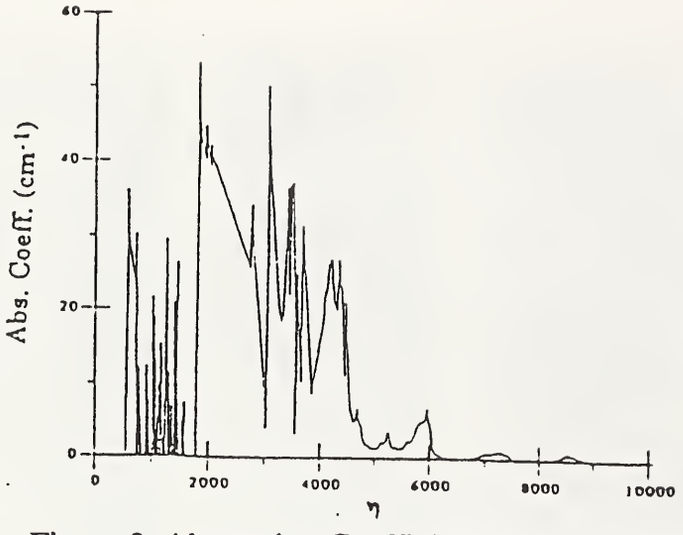


Figure 2. Absorption Coefficient (cm-1) against wavenumber (cm-1) for clear PMMA

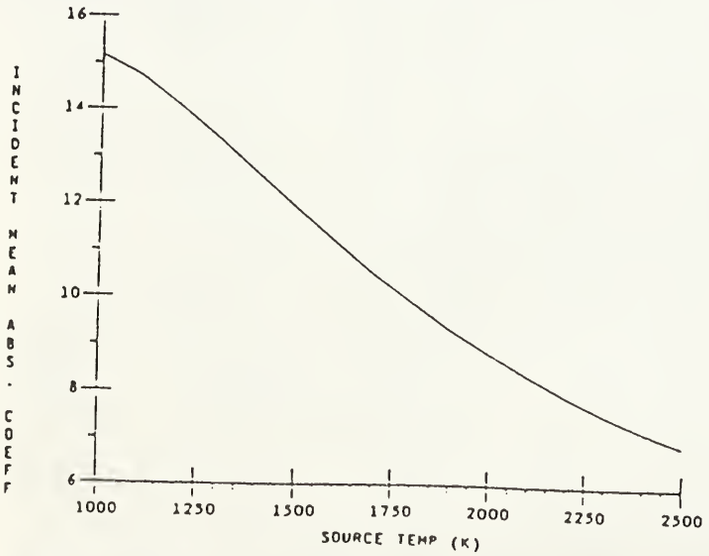


Figure 3. Planck Mean or Incident Mean Absorption Coefficient Against Black Body Source Temperature for PMMA

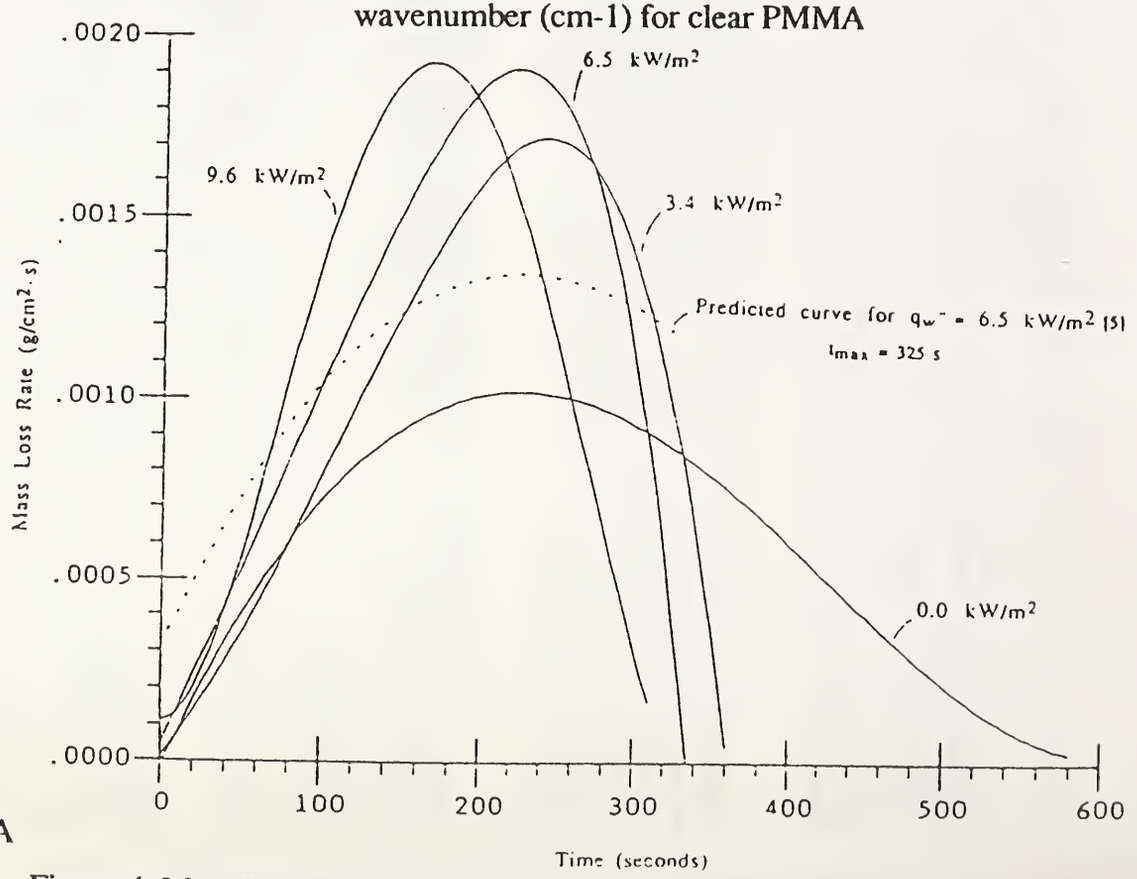


Figure 4. Mass Loss Rate at Various Levels of External Radiation for Masonite

1.8 Fire Supppression

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - 1991

FIRE SUPPRESSION

Professional Staff: David D. Evans, Project Leader
William D. Walton, Fire Protection Engineer
Kathy A. Notarianni, Fire Protection Engineer
Daniel Madrzykowski, Mechanical Engineer
Arvind Atreya, Visiting Faculty

Project Objective:

Determine and scope by August 1991, the use of new technology to enable breakthroughs in National fire suppression capabilities resulting in significant reduction in the loss and cost of fire.

Scope:

Perform an assessment of the ultimate performance that can be expected from suppression systems utilizing existing agents and possible new agents and hardware.

Technical Accomplishment:

Utilizing results from the last few years of both STRS and other agency fire suppression research, a fire suppression module for HAZARD has been designed to enable users to calculate the benefit of sprinklers in the hazard assessment. The module contains both zeroth and first order models for burning rate reduction after calculated sprinkler actuation. This module will be included in the next release of HAZARD.

The long range plan for fire suppression research at NIST was formulated to de-emphasize the short term support of technology for existing suppression systems in favor of using the limited resources available to explore means to enable a new generation of fire suppression equipment and agents. The plan focuses on the development of a rigorous means to measure the effectiveness of suppressants and the speed of fire suppression. Measurements based on the effects of agents on a axisymmetric diffusion flame are proposed as the best vehicle for experimental control and ease of prediction.

Funding was reprogrammed from the planned measurement of CO_2 dispersion in an enclosure and time dependent concentration prediction using the Harwell FLOW3D model to support measurement efforts on the Kuwait fires.

Publications :

"The Reduction in Fire Hazard in Corridors and Adjoining Corridors Provided by Sprinklers," D. Madrzykowski, NISTIR 4631, (1991).

"Suppression of Post-Flashover Compartment Fires Using Manually Applied Water Sprays," D. W. Stroup, and D. D. Evans, NISTIR 4625, (1991).

"Development of A Sprinkler Effectiveness Methodology for the GSA Engineering Fire Assessment System," D. Madrzykowski, and R. Vettori, NISTIR in preparation.

"Temperature and Radiation of Diffusion Flames with Suppression," J. P. Gore, D. D. Evans, and B. J. McCaffrey, Combustion Science and Technology, Vol 77, pp. 189-202, (1991).

"Five Small Flaming Fire Tests in a Simulated Hospital Patient Room Protected by Automatic Fire Sprinklers," K. A. Notarianni, NIST REPORT OF TEST FR 3982, (October 31, 1991).

Related Grants:

"Extinguishment of Combustible Porous Solids by Water Droplets," Arvind Atreya, Michigan State University.

"Transient Confined Ceiling-Jet Characteristics in the Presence of an Upper Layer," Vahid Motevalli, Worcester Polytechnic Institute.

"Transient Cooling of a Hot Surface by Droplets Evaporation," Marino DiMarzo, University of Maryland.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 91

Institution:	Michigan State University
Grant Number:	60NANB8D0861
Title:	Extinguishment of Combustible Porous Solids by Water Droplets
Principal Investigators:	Arvind Atreya & Indrek S. Wichman Department of Mechanical Engineering Michigan State University East Lansing, MI 48824
Other Professional Personnel:	Peter Caffrey (M. S. candidate)
NIST Scientific Officer:	Dr. David D. Evans

TECHNICAL ABSTRACT:

This work is focused on cooling and extinguishment of combustible porous solids by water droplets. The objective is to quantify the rate of suppression as measured by the decrease in the energy release rate from the porous solid during a fire due to water application and the eventual time to extinguishment. Although this work is oriented purely toward the condensed-phase suppression action by pure water droplets, it provides a standard for comparison with other suppression agents and methods.

During the current fiscal year, progress was made on the following topics: (i) Completion of the design and construction of the stagnation point flow apparatus. (ii) Preliminary testing and modification of the apparatus using PMMA samples. (iii) Obtaining some preliminary results for PMMA. (iv) Completion of experimental and theoretical work regarding our previous study on piloted ignition (while this was not proposed in the current contract year, one of the students working on the project had not yet completed his Ph. D. thesis). Two papers were written based on this work. One of these papers will be presented in the Third International Fire Safety Science Symposium while the other will be submitted to Combustion and Flame. These are entitled: (a) Effect of environmental variables on Piloted Ignition, and (b) A Theoretical Investigation of Piloted Ignition of Wood.

The Suppression Apparatus:

The apparatus designed for suppression studies is schematically shown in Figure 1. It consists of a cylindrical 1200 °C furnace (approximately 20" tall) with a center ceramic tube for gas supply/exhaust. This ceramic tube supports a ceramic honeycomb heat exchanger and a ceramic honeycomb flow straightener. The entire furnace is supported by a specially designed ceramic flange which is supported by a water-cooled stainless-steel cylinder which hangs from a water-cooled circular aluminum plate. An outer concentric stainless-steel casing is used to direct the exhaust gases through the annular opening B. A 12" diameter quartz glass tube that can slide over the stainless-steel casing is used as an observation window. This glass tube sits on a soft silicone foam rubber support to prevent gas leakage. The cylindrical sample which sits on a scale (for weight measurements) is surrounded by ceramic insulation to ensure one-dimensional heat conduction. The entire bottom sample assembly is also supported by a water-cooled circular aluminum plate. A chrome-plated water-cooled droplet tube that can swing in and out of the hot burner zone is used to release water droplets on the sample surface.

Prior to conducting the experiments, the water-cooled radiation shield protects the sample from the furnace radiation. The experiment begins when this radiation shield is removed. Measurements show that up to 4 W/cm^2 can be obtained on the sample surface in this configuration with a 5% non-uniformity. The furnace heaters are electrically controlled and permit the control of external radiation on the sample surface. This apparatus also permits the control of composition, temperature, velocity and direction of gas flow. It permits transient measurements of exhaust gas composition, sample weight loss and temperatures both with and without the application of the suppression agent. A video camera is used to continuously record the extinguishment history. A computer analysis of this record photographically measures the reduction in the flame size and intensity as well as the time to extinguishment.

Results

When a water droplet falls on the surface of a burning sample it quenches the production of fuel gases and produces water vapor instead. The net effect of this action on the stagnation point diffusion flame is to punch a hole in the flame. The size of this hole is a measure of the droplet influence on the flame. Larger the droplet, larger is the influence area as shown in Figure 2. It is also clear from Figure 2 that the influence radius is much larger than the droplet radius and that the relationship is nonlinear [Note that the quantitative determination of this effect is possible because of the chosen flame geometry]. Due to this extinguished zone inside the flame, the heat feedback form the flame to the solid reduces resulting in lower fuel production. For a small sample and under low external radiation conditions, comparatively large droplets more frequently applied lead to extinguishment.

These experimental results lead to a qualitative suppression diagram presented in Figure 3 for PMMA in the stagnation-point-flow apparatus. Here the non-dimensional drop density is defined as:

$$\textit{Non-dimensional drop density} = \frac{\textit{Sample surface area}}{\textit{Droplet influence area X \# of drops}}$$

and the non-dimensional external heat flux as:

$$\textit{Non-dimensional heat flux} = \frac{\textit{(External flux - Minimum flux at ignition) X Area}}{\textit{(Droplet mass X Heat of evaporation X Drop frequency)}}$$

In defining the non-dimensional droplet density in Figure 3 the droplet diameter was used to calculate the influence area. Of course, as can be seen from Figure 2, the actual influence area is much larger. However, this was not used in order to separate the effects.

Figures 4 and 5 show the results of overall species composition measurements obtained in the exhaust port B of Figure 1. These measurements will be used to calculate the effect of water droplets (or other suppression agents) on the overall heat release rate. As can be seen from Figure 4, our measurements do not seem to reach a steady horizontal asymptote (as would be expected), instead they show significant fluctuations. These fluctuations are because the sample had to be moved up to maintain a constant level (see Figure 1) and the device used to accomplish this was a lab jack which is quite unstable. This problem is being corrected. Yet, it is encouraging to note that the effect of water droplets can be easily measured and that it is substantial specially prior to extinguishment (Figure 5). Such measurements will be conducted for other suppression agents as well.

Reports and Papers:

1. Tzeng, L. S.,"Theoretical Investigation of Piloted Ignition of Wood," Ph.D Thesis, Michigan State University, 1990.

2. Abu-Zaid, M. , "Effect of Water on Ignition of Cellulosic Materials," Ph.D Thesis, Michigan State University, 1988. Also published as NIST-GCR-89-561, 1989.

3. Tzeng, L. S., Atreya, A., and Wichman, I. S., "A One-Dimensional Model of Piloted Ignition," Combustion and Flame, 1990.

4. Atreya, A., and Abu-Zaid, M., "Effect of Environmental Variables on Piloted Ignition," Third International Fire Safety Science Symposium, 1991.

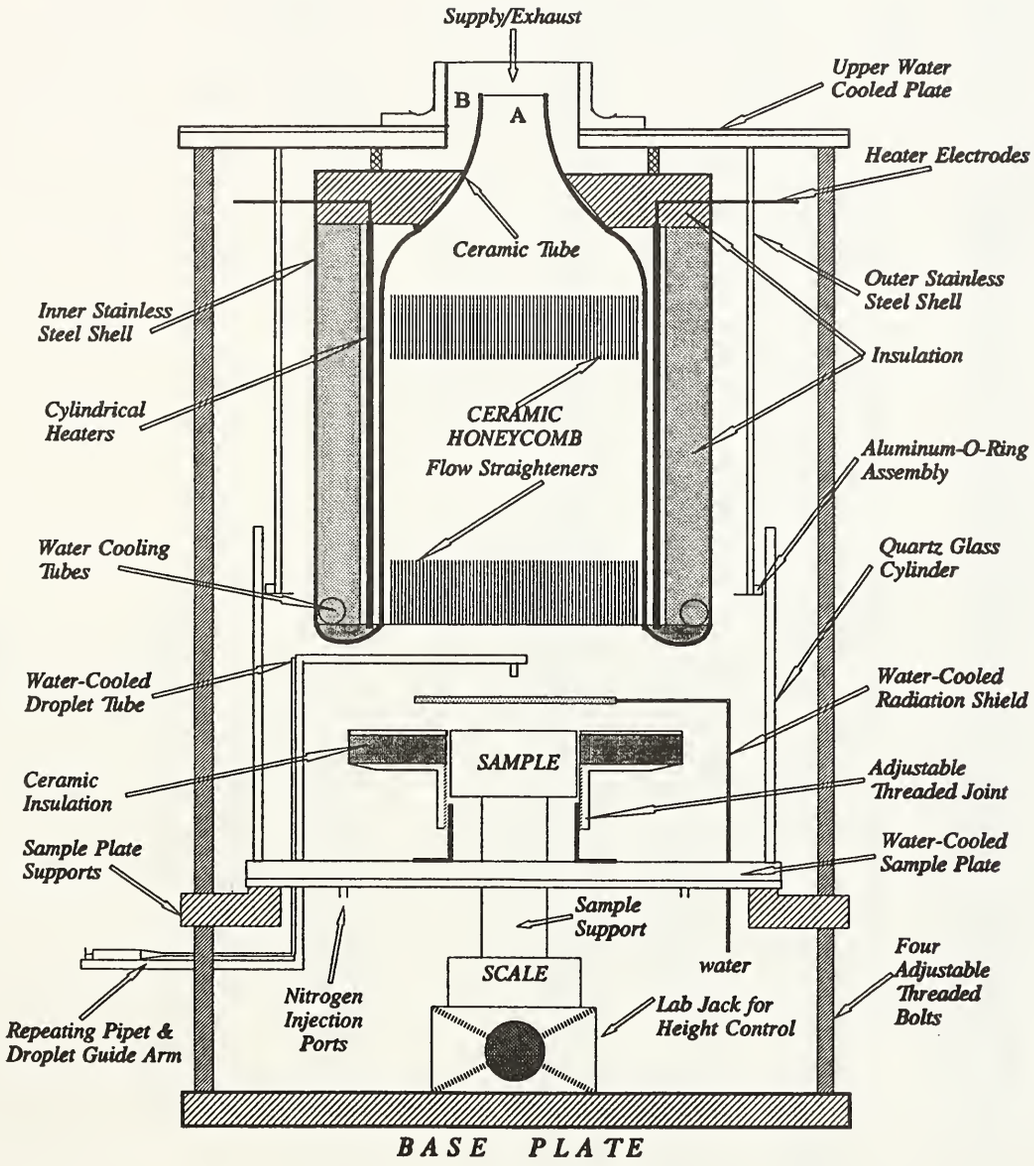


Figure: 1 Stagnation Point Flow Apparatus for Suppression Studies.

FIGURE 2 : DROPLET FLAME INFLUENCE RADIUS FOR VARIOUS SIZE DROPLETS.

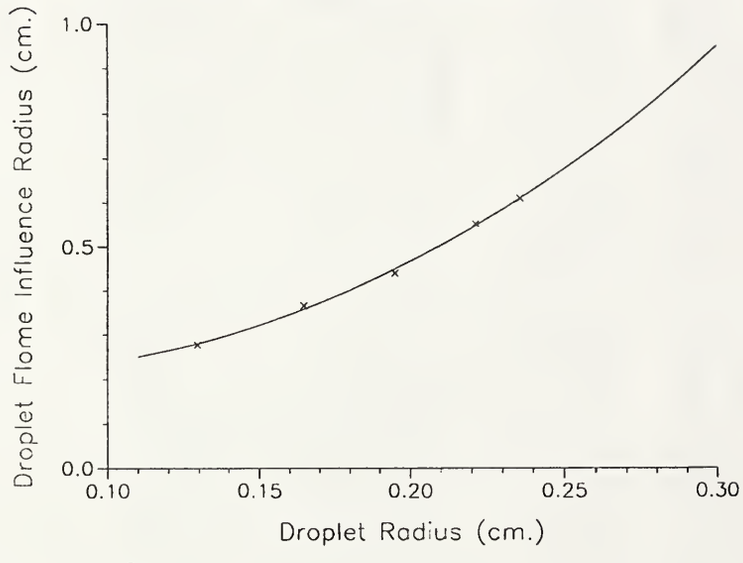


FIGURE 3 : MEASUREMENTS OF THE SUPPRESSION CURVE FOR PMMA IN THE STAGNATION FLOW APPARATUS.

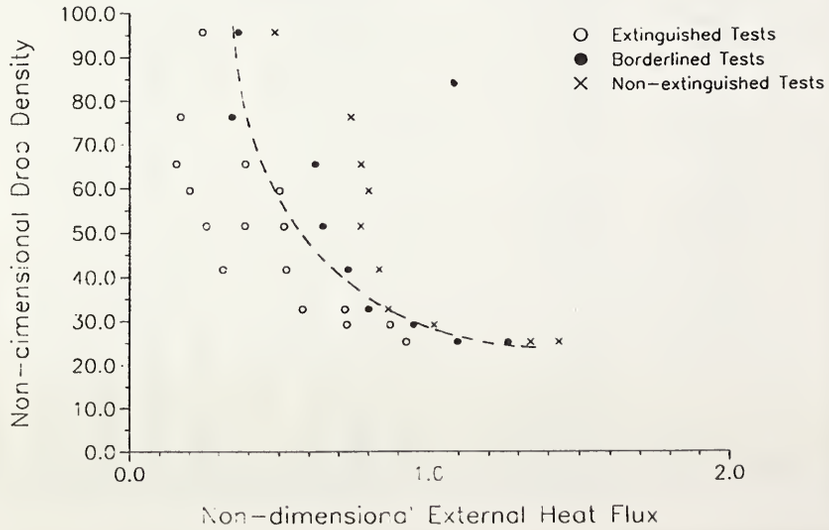


FIGURE 4: HEAT RELEASE RATE MEASUREMENTS DURING WATER DROPLET APPLICATION.

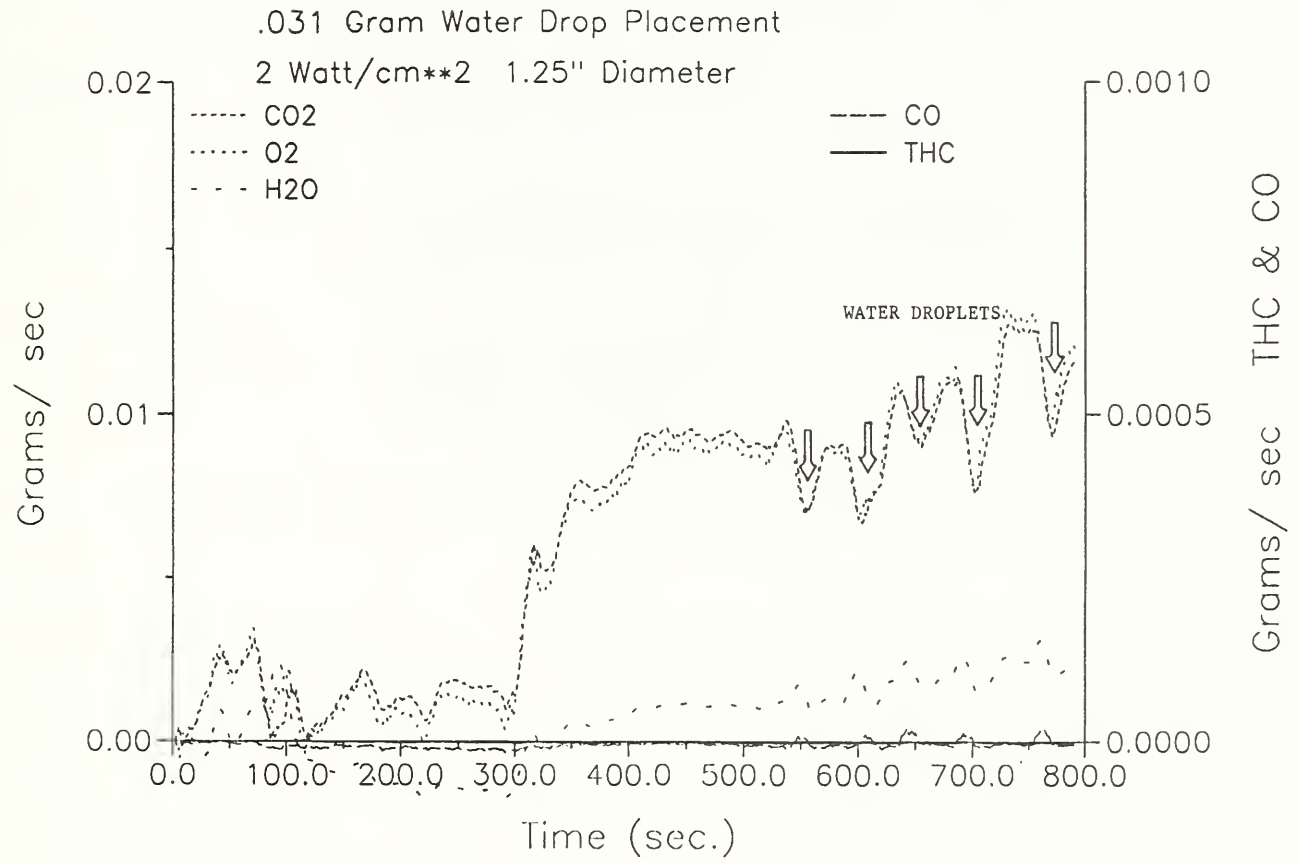
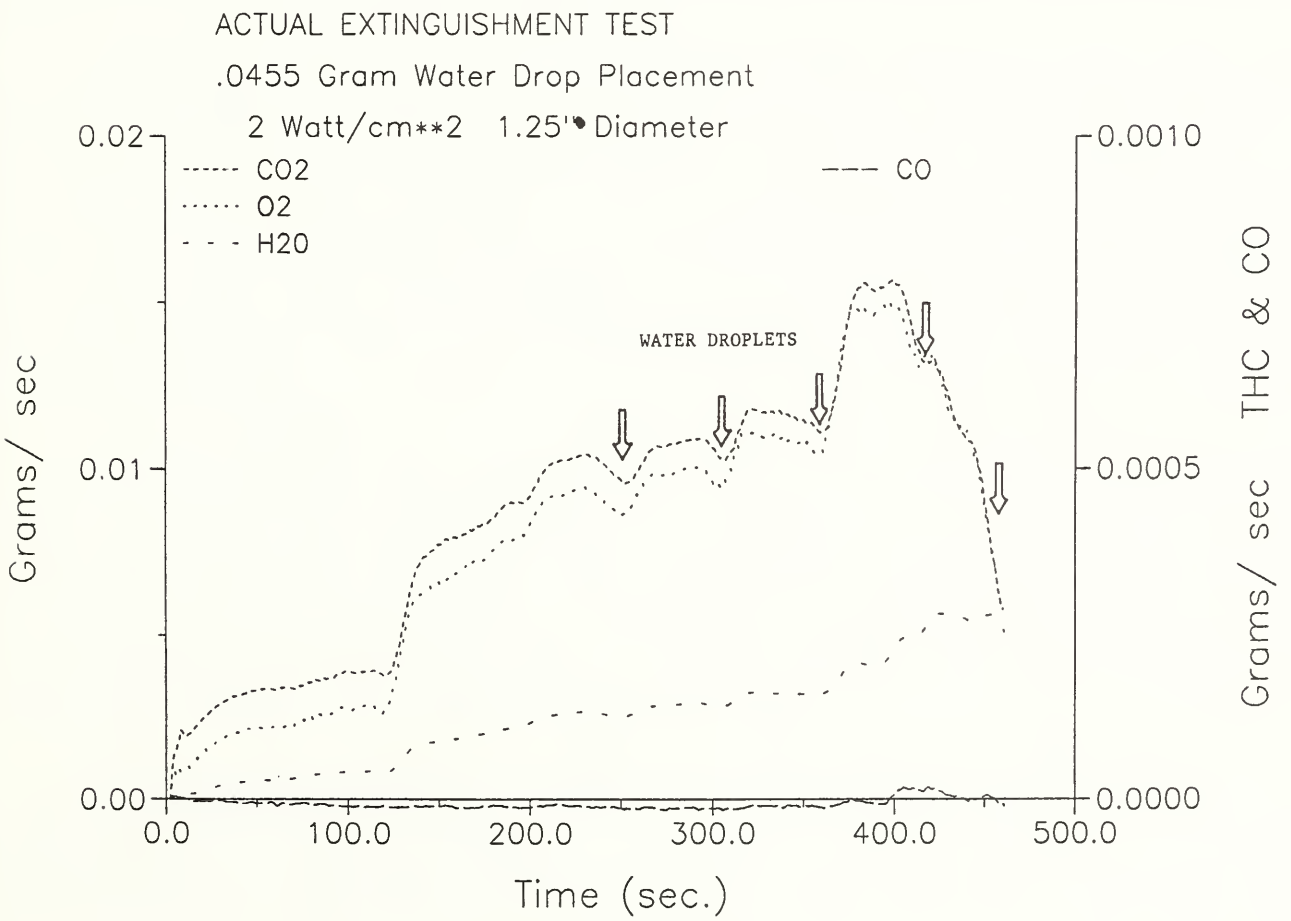


FIGURE 5: HEAT RELEASE RATE MEASUREMENTS DURING WATER DROPLET APPLICATION -- LEADING TO EXTINGUISHMENT.



BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

Institution: Worcester Polytechnic Institute

Grant No: 60NANBOD1049

Grant Title: **Transient Confined Ceiling Jet Characteristics in the Presence of an Upper Layer**

Principal Investigator: Professor Vahid Motevalli
Center for Firesafety Studies
Worcester Polytechnic Institute
Worcester, MA 01609

Other Professional Personnel: Christina Ricciuti, Graduate Student

NIST Scientific Officer: Dr. James Morehart

Introduction The development of an upper layer in an enclosure fire is thought to have notable effects on the ceiling jet. The presence of this hot gas layer increases the temperature in the ceiling jet and the heat transfer to the ceiling. Accurate prediction of the characteristics of the confined ceiling jet is important in calculating the time to operation of detection and suppression devices and for fire modeling purposes. The data presented here represents a collection of transient and steady-state temperature and velocity measurements of a confined ceiling jet and upper layer. The results from this data were compared to experimental data collected by Motevalli and Marks [1] for unconfined ceiling jets using the same apparatus. The main objective of this work was to develop a better understanding of the characteristics of the confined ceiling jet in the presence of an upper layer. This was accomplished through comparison of the confined and unconfined ceiling jet data, quantification of the developing upper layer and analysis of heat transfer to the ceiling.

Description of the Problem In the case of an unconfined ceiling jet, the jet flows along the ceiling entraining the enclosure's cooler ambient air and transferring heat to the ceiling. The ceiling jet grows in thickness as the temperature and velocity decrease. In an enclosure (confined conditions) this jet will be forced to turn downward when the flow encounters a wall, forming an upper layer of hot gases and fire products. As the upper layer forms, it effects the characteristics of the ceiling jet and portion of the plume contained in the upper layer. The plume and ensuing ceiling jet contained in the upper layer have a lower momentum and an increased temperature. These effects on the ceiling jet need to be closely examined and quantified to define the confined ceiling jets characteristics. Quantification of the ceiling jet is attempted here through analysis of the confined ceiling jet velocity and temperature and comparison with the unconfined data.

Objectives This study was concerned with the characteristics of the confined ceiling jet in the presence of an upper layer, the transient development of this layer and the comparison of these charachteristics to the unconfined ceiling jet. Three specific objectives were addressed in this work. The first objective was to compare and analyze the data for the confined ceiling with the correlations obtained from the unconfined ceiling and to determine differences in the characteristics of the ceiling jet due to the effect of the upper layer development. The second objective was to quantify the transient and steady-state characteristics of the ceiling jet and development of the upper layer. The third objective was to analyze the heat transfer from the ceiling jet to the ceiling.

Experimental Apparatus The apparatus used for the confined ceiling experiments was the same as that used in the unconfined ceiling jet studies of Motevalli and Marks and is shown in Figure 1 except with an added curtain wall to model an enclosure. The depth of the curtain wall, z, was 0.5 meters with a ceiling height, H, of 1.0 meter, (thus, the distance between the floor and the bottom of the curtain wall, $Z = 0.5$). The ceiling was constructed of 1.27 centimeter thick fiberboard with a measured emissivity of

0.9. The ceiling was insulated on the back side with 8.26 centimeter thick layer of standard fiberglass insulation, (R-11). The curtain walls were constructed of corrugated cardboard and also insulated. The fire was produced using a burner fed by premixed methane and air at stoichiometric conditions. Steady fires with heat release rates of 0.75 and 2.0 kilowatts were used in these experiments.

Results Temperature profiles were recorded for the confined ceiling jet and the upper layer for the 2.0 and 0.75 kilowatt fire at radial locations of 0.26 and 0.75 meters. Velocity profiles were recorded for the 2.0 kilowatt fire at radial locations of 0.26 and 0.75. Figure 2 shows the velocity profiles for confined and unconfined ceiling jet for the 2.0 kW fire at r/H of 0.26 at times of 5 seconds and steady state. At 5 seconds the confined ceiling jet has not been affected by the developing upper layer. This profile closely resembles the unconfined ceiling jet profiles. At thirty seconds into the fire the upper layer has developed enough to significantly alter the confined ceiling jet velocity. This velocity is considered to be steady at this point. Figure 2 also demonstrates the difference in maximum velocities at steady-state. The presence of the upper layer reduced the maximum velocity by 25%.

Figure 3 shows the development of the temperature profiles for the ceiling jet and upper layer for the 2.0 kW fire at r/H of 0.26. The bottom of the curtain wall is located at z = 50 cm. A distinct ceiling jet profile is evident in the upper layer, even at steady-state. The average upper layer temperature is only

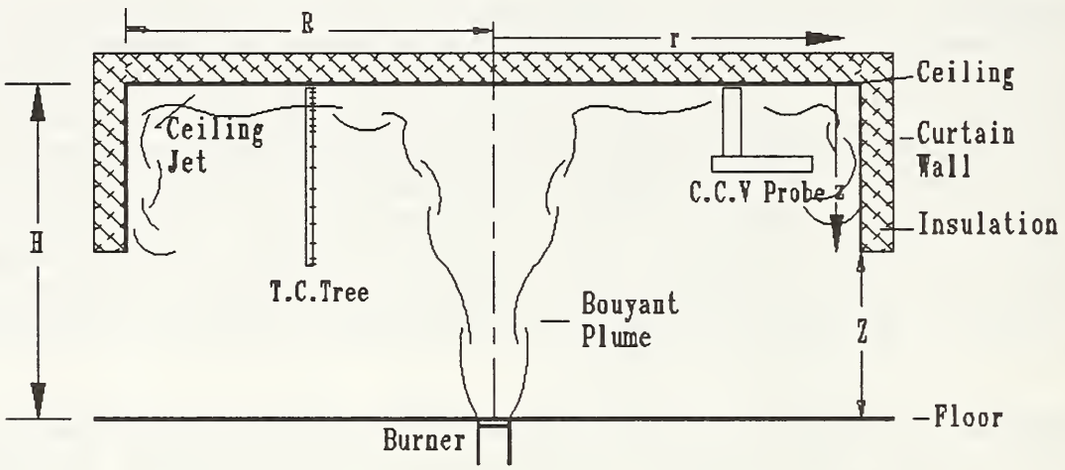


Figure 1 - Experimental Apparatus for Confined Ceiling

1/2 to 2/3 of the maximum ceiling jet temperature. This figure shows the quick development of the upper layer. After 4 minutes, the upper layer temperature has reached 80-90% of the steady-state maximum temperature. Figure 4 is a comparison of the confined and unconfined ceiling jet temperature at 30 seconds into the fire. This figure shows that even during the very early times the unconfined ceiling jet does not correlate with the confined ceiling jet. The ceiling jet for the unconfined and confined situations have the same thickness but the maximum temperature in the confined jet is farther from the ceiling. The maximum jet temperature was normalized using the expression shown below and plotted in Figure 5.

$$\Delta T^{*}_{max} = \frac{\Delta T_{max}}{Q^{*2/3} T_{\infty}} \qquad (1)$$

Time was first is normalized by an experimentally determined time constant, τ, which is equal to the time at which $\Delta T/\Delta T_{max} = 1\text{-}1/e$. Dimensional analysis of the energy balance of the upper layer results in the relation similar to that obtained by Veldman et al.:

$$\tau = \frac{\rho_{\infty} c_{\infty}}{\rho_c c_c} \frac{\sqrt{gH}}{\delta} Q^{*-1/3} f(r/H)^{-1} \qquad (2)$$

where the ceiling properties are subscripted by c and ceiling thickness is δ.
Using this time constant seem to correlate the data just as well as the experimental τ. A fit to the data in Figure 5 provides a prediction of the maximum temperature in the ceiling jet as a function of time when fire size and radial location is known.

$$\frac{\Delta T^*_{max}}{f\,(r/H)} = 1 - e^{\left(-0.01\frac{t}{\tau}\right)} \qquad (3)$$

where f(r/H) is a linear function since data from only two r/H locations were available.

The average upper layer was found to be a function of fire size only and not r/H. Figure 6 shows the average upper layer temperature normalized by fire size and ambient temperature and time normalized by τ from Veldman et al. A curve fit to the experimental data predicts the average upper layer temperature as a function of t/τ.

$$\Delta T^*_{avg} = (7.1 + 0.0045(t/\tau))\ (1 - e^{t/\tau}) \qquad (4)$$

The transient convective heat transfer coefficient to the ceiling, h_c, was determined using the energy balance at the ceiling surface and a numerical solution of the one-dimensional transient conduction into the ceiling. The values for h_c were between 4.0-6.0 W/m^2 K for the 2.0 kW fire size.

Conclusions The results demonstrated that the upper layer affected the ceiling jet almost immediately. The confined ceiling jet demonstrated a higher temperature and reduced velocity caused by the upper layer. Correlations for the unconfined ceiling jet were found to be ineffective in predicting the characteristics of the confined ceiling jet. Transient maximum ceiling jet temperature and average upper layer temperatures were correlated as a function of time. Heat transfer analysis showed convective coefficients lower than theoretical studies.

Reports and Papers

1. Motevalli V. and Ricciuti, C., "Characterization of the Confined Ceiling Jet in the Presence of an Upper Layer in Transient and Steady-State Conditions", Final Report to NIST, July 1991.
2. Ricciuti, C. and Motevalli, V., "Characteristics of Confined Fire-Plume_Driven Ceiling Jets", Eastern Section of the Combustion Institute, Dec. 1990, Orlando, Fl.
3. Ricciuti, C. and Motevalli, V., "Transient Confined Ceiling Jet Characteristics in the Presence of an Upper Layer", Eastern Section of the Combustion Institute, Oct. 1991, Ithaca, NY.

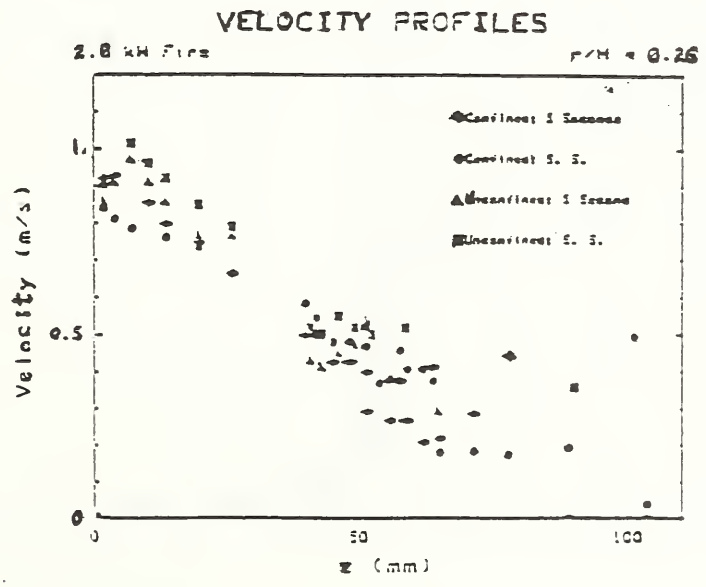


Figure 2 - Velocity Profile, Confined vs. Unconfined

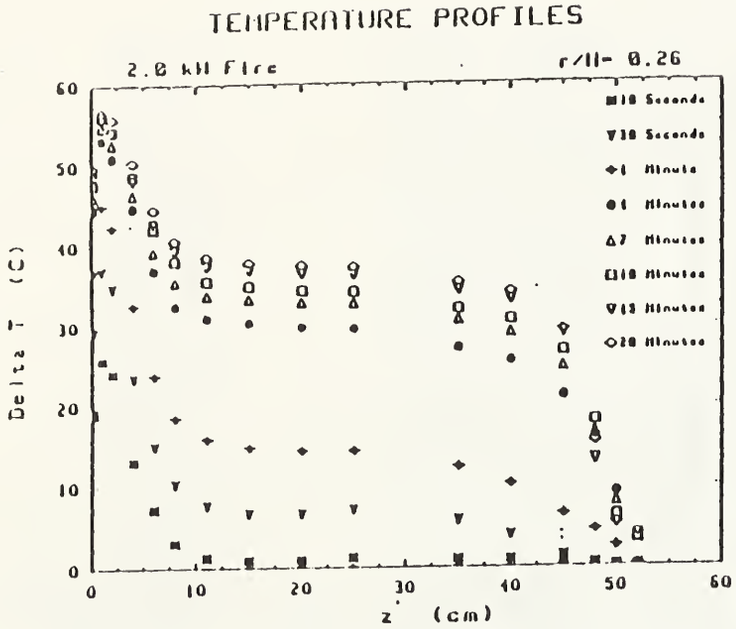


Figure 3 - Upper Layer Temperature Profile

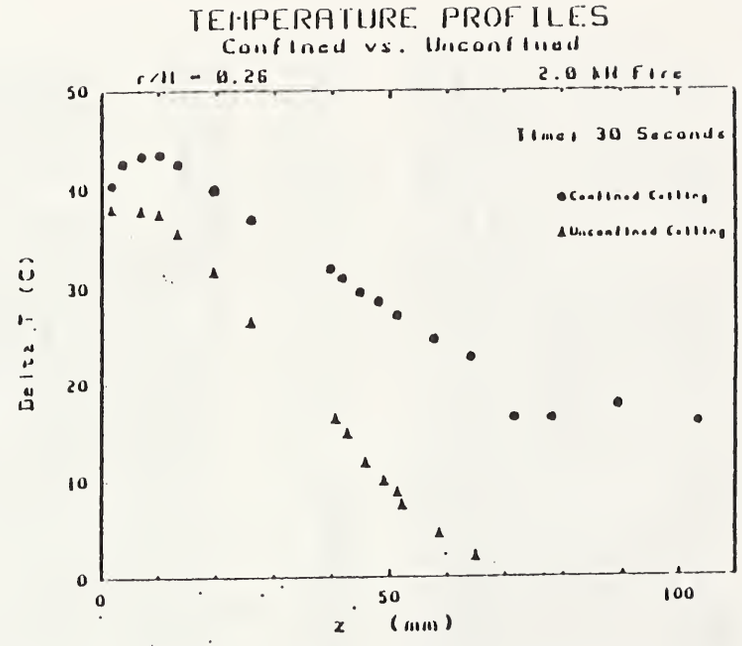


Figure 4 - Confined vs. Unconfined Ceiling Jet Temperature

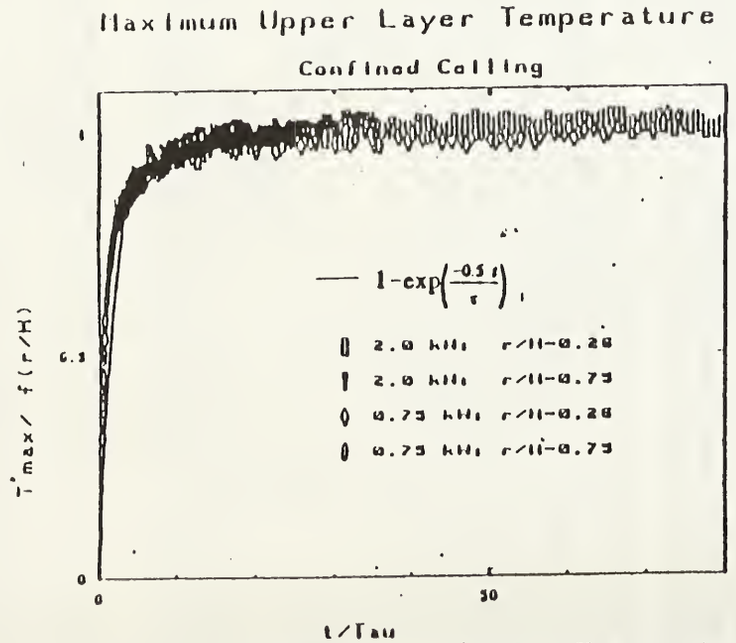


Figure 5 - Maximum Ceiling Jet Temperature

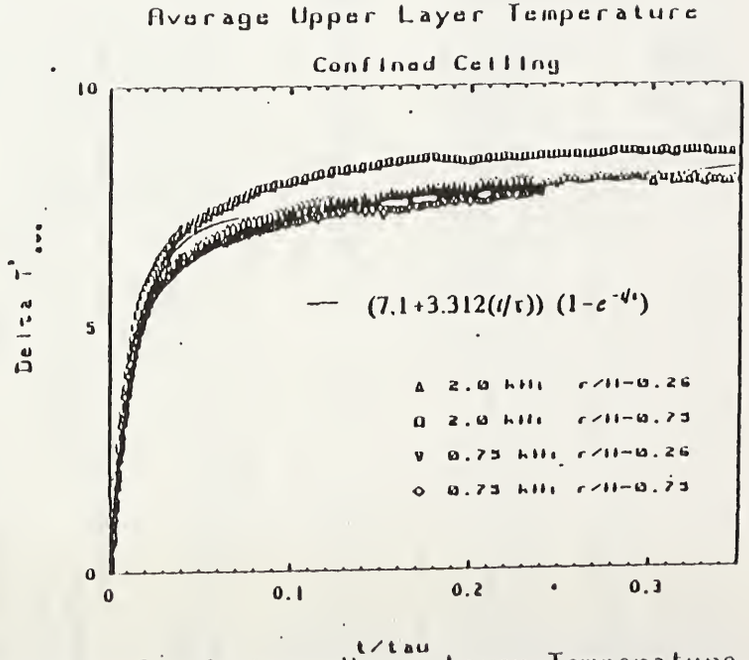


Figure 6 - Average Upper Layer Temperature

BUILDING AND FIRE RESEARCH LABORATORY
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NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution: University of Maryland

Grant No: 70NANB8H0840,3

Grant Title: Transient Cooling of a Hot Surface by Droplets Evaporation

Principal Investigator: Dr. Marino di Marzo
Mechanical Engineering Department
University of Maryland
College Park, MD 20742

Other Personnel: H. Dawson, Graduate Student
C. Kidder, Graduate Student
Y. Liao, Doctoral Student
P. Tartarini, Doctoral Student

NIST Scientific Officer: Dr. David D. Evans

Technical Abstract:

Introduction. The phenomena associated with solid fuel fire extinguishment processes are related to the evaporation of water droplets deposited on hot solid surfaces. A single droplet model is obtained which predicts the behavior of single droplets deposited on a hot, non-porous solid material. The predictions of this single droplet model are successfully incorporated in a multi-droplet model which predicts the cooling effect of a spray. This information is for a solid heated from below by conduction. A more realistic scenario is used to gather experimental data concerning droplet evaporative cooling in a fire environment. Single droplet evaporative cooling behavior for the case of a solid heated from above by radiation is studied experimentally and an extensive data base is gathered to validate the prediction of a model which will include radiative heat input.

Evaporative Cooling With Radiant Heat Input. An extensive data base is compiled for droplets deposited on Macor (a glass-like material). A Macor tile is heated from above by two radiant heaters similar in configuration to the cone calorimeter. The tile is also cooled on its lower surface to establish a strong one-dimensional heat transfer pattern in the vertical direction and to minimize the edge effects. This initial steady state is altered locally by the introduction of a water droplet at the center of the exposed face of the tile. The droplet initial volume spans from 0.05 ml to 0.01 ml. The tile is 2.54 cm thick and it is square in shape with 15.24 cm sides. The droplet is deposited by a mechanical device which insures a high degree of repeatability. Each test is repeated ten times to yield consistency

in the measurements. Surface preparation, water degassing, calibration of the measuring apparatus are repeatedly checked to provide high confidence in the experimental information.

The evaporative process is monitored by infrared thermography. Particular care is used to shield the infrared camera from direct or reflected radiation from the heaters. A chilled pipe is used to bound the camera field of view to the portion of the solid surface of concern. The infrared signal is calibrated and referenced to a surface reading obtained with a thermocouple surface probe. The data are available as a vcr tape which shows the transient temperature profile over a line passing through the center of the solid surface wetted region. This information is scanned and converted into a matrix that associates an intensity to each location in the temperature-space plane. The matrix is binarized with a tresholding technique and both noise and reference isothermal lines are eliminated from the record. Finally a curve fit of the pertinent information is obtained and an ASCII file containing temperature versus location is obtained. This process is repeated at various times during the evaporative process and for each drop size and initial solid surface temperature. The date base along with all the necessary information is available on PC diskettes.

The most notable difference with the conduction case (where the solid is heated from below) is in the behavior of the shape parameter. Figure 1 shows that the shape parameter increases with the initial solid surface temperature whereas for the conduction case its value is virtually constant. This is due to the direct radiant heat input into the exposed surface of the droplet, which affects the surface tension and thus the shape of the deposited droplet. Radiation is directly evaporating the water and indirectly supplying heat through the solid at the solid-liquid interface. The contribution to evaporation by conduction is reduced with respect to the pure conduction case. This is quite intuitive if one considers that while the droplet deposited on the solid heated from below causes a sharp increase in the axial temperature gradient, the same droplet is sharply reducing such gradients in the radiative case. Further, the heat input to the surface available for the droplet evaporation is channeled through a shallow portion of the solid near its surface. In summary, the increased direct radiant input is offset by the reduced conduction contribution to yield evaporation times comparable to the one observed for the pure conduction case. It turns out that overall the evaporation is about ten per cent faster for the radiative case. The detailed partitioning of the energy contribution to the evaporative phenomena will be assessed with a detailed simulation code which is based on the previously validated conduction code.

Multi-Droplet Simulation. The prediction of the single droplet model developed for the conduction case constitutes the basis for a multi-droplet code. This code is based on the superposition of the cooling effects of all the droplets deposited on the surface with respect to the portion of the surface under consideration. The overall surface about a particular point is partitioned in a near field and in a far field. The effect of droplets deposited in the near field is obtained from multi-dimensional arrays which are compiled with the single droplet solution. The effects of droplets deposited in the far field is obtained with a simple analytical exact solution which represents the droplet as a point source while satisfying the energy inventory. A small portion of the overall surface subjected to the droplet spray is considered and a three dimensional plot of its transient thermal evolution is depicted in

Figure 2. On the right hand side of the figure, the average sample surface temperature is plotted as a function of time and an exponential curve is fitted to these data.

Note that this particular simulation is executed with droplets of 0.005 ml with a mass flux of 0.016 Kg/m^2s. A typical sprinkler mass flux is about three times as large with an average droplet volume of about 0.001 ml. For this case all the droplets are identical and they are gently deposited on the surface in a random fashion. Each droplet evolves in accordance to the initial solid surface temperature corresponding to the local surface temperature at the site and instant of deposition.

The same multi-droplet code will be used with the results obtained by the single droplet code developed for the radiative heat input from above the surface and its results will be validated against experimental data for multi-droplet cooling with similar radiative heat input which are currently under way. The final product of this research will be a model which will predict extinguishment and exposed surface cooling in a fire environment. A simplified version of the algorithm will be designed for inclusion in the existing codes.

Acknowledgements. The authors are indebted to Dr. H. Baum (NIST) for his guidance on the development of the multi-droplets code.

Reports and Papers:

1. M. Klassen, M. diMarzo, J. Sirkis, "Infrared Thermography of Dropwise Evaporative Cooling" Experimental Thermal and Fluid Science, submitted, 1991.

2. P. Tartarini, Y. Liao, M. diMarzo, "Transient Cooling of a Hot Surface by Droplets Evaporation", Mechanical Engineering Department Report, No. 90-6, University of Maryland, 1990

3. C. Kidder, "Dropwise Evaporative Cooling of a Ceramic Solid Surface Heated by Radiation", Master of Science, 1990.

4. M. diMarzo, Y. Liao, P. Tartarini, D. Evans, H. Baum," Dropwise Evaporative Cooling of a Low Thermal Conductivity Solid", 3rd IAFSS International Symposium on Fire Safety Science, Edinburgh (UK), in press, 1991

5. M. diMarzo, P. Tartarini, Y. Liao, D. Evans, H. Baum, "Dropwise Evaporative Cooling", Proceedings of the 28th ASME/AIChE/ANS/AIAA National Heat Transfer Conference, HTD-Vol. 166, pp. 51-58, 1991

6. P. Tartarini, M. diMarzo, "The Solid-Liquid Interfacial Conditions for Dropwise Evaporative Cooling", Proceedings of the 9th UIT National Heat Transfer Conference, Pisa (Italy), pp. 61-75, 1991

7. M. diMarzo, P. Tartarini, Y. Liao, D. Evans, H. Baum, "Dropwise Evaporative Cooling", ASME Journal of Heat Transfer, submitted, 1991

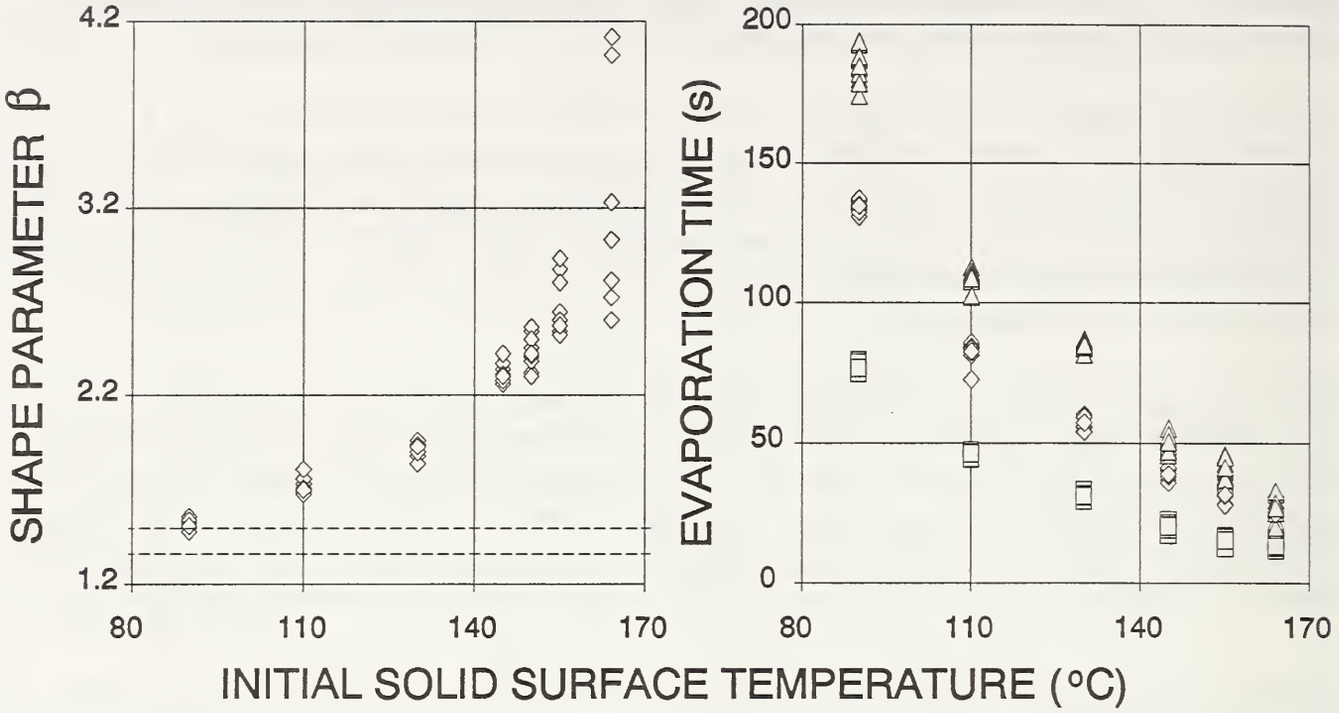

FIGURE 1: Shape parameter and evaporation time for various droplet sizes and initial solid surface temperatures (△ - 0.05 ml; ◇- 0.03 ml; □- 0.01 ml). The dashed lines in the left hand side plot bound the typical shape parameter values for the conduction case.

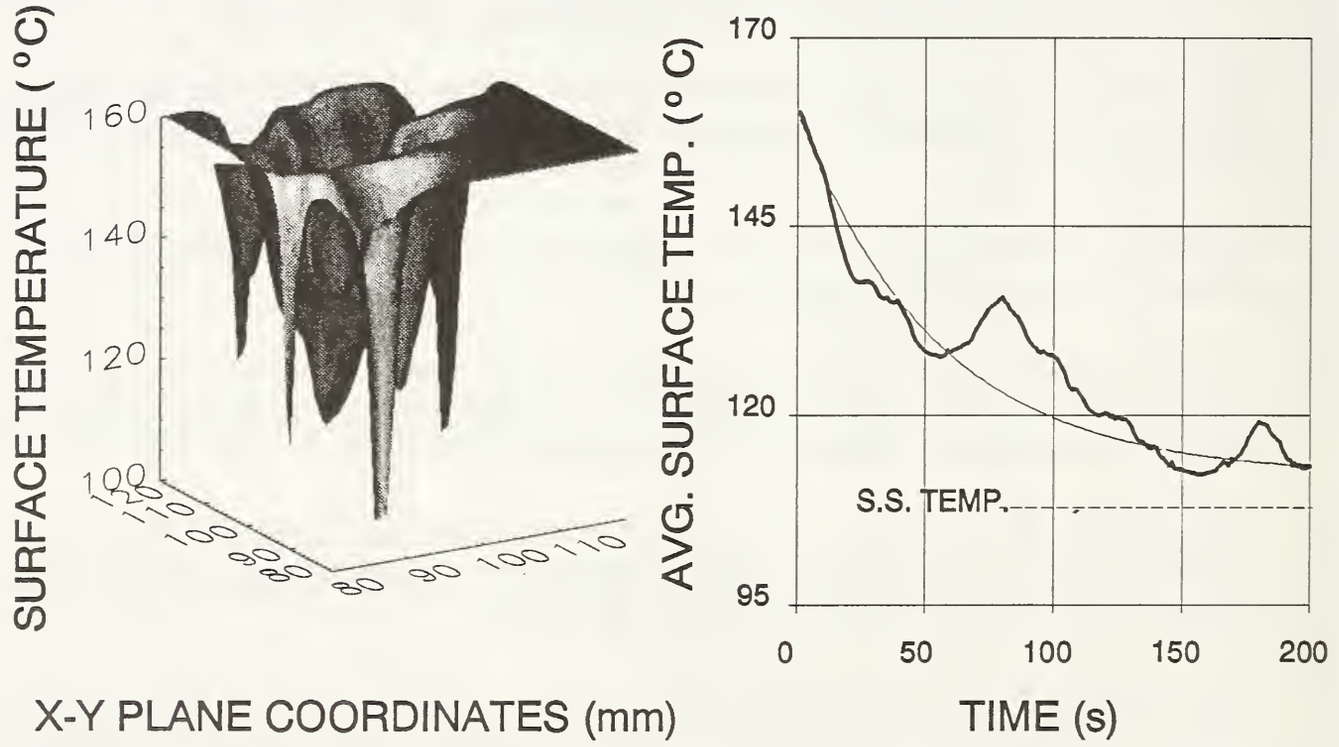

FIGURE 2: Instantaneous surface temperature distribution over a 6x6 cm area subjected to a 20 cm diameter spray of 0.005 ml droplets with a mass flux of 0.016 kg/m^{2}s. The right hand side shows the average surface temperature as a function of time (time to reach steady state is ~ 370 s).

1.9 Fire Hazard Assessment

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT – 1991

CONE CALORIMETER AND LIFT SUPPORT

Professional Personnel

Vytenis Babrauskas, Project Leader
Katie Chartier, Research Associate, Isover Saint Gobain CRIR
Marc Janssens, Research Associate, National Forest Products Association

Project Objective

To provide a limited amount of user support for the Cone Calorimeter and the LIFT apparatus during FY91; to maintain the CFR apparatus during FY91 and to make necessary minor upgrades.

Scope

The areas of work for FY91 included: Progress Cone and LIFT methods in ISO standardization and in ASTM balloting. Make needed repairs. Assist users with problems and applications. Participate in Cone Calorimeter round robins for both ASTM and ISO. Organize Cone Calorimeter workshops.

Technical Accomplishments

The world population of Cone Calorimeters reached about 70.

A revised Cone Calorimeter standard was issued by ASTM, incorporating repeatability and reproducibility data obtained from round robin testing.

The ISO Draft International Standard on the Cone Calorimeter was approved to be issued as an International Standard.

The U.S. Navy issued a specification based on Cone Calorimeter testing.

The Second International Conference on Heat Release was organized, held Feb. 27-28, 1991 in Brussels, Belgium.

The First U.S. Symposium on Heat Release and Fire Hazard has been organized and will be held in San Diego on Dec. 12-13, 1991.

A study was conducted on the effects of edge frames and other different sample edge conditions for Cone Calorimeter samples. This study will result in recommendations being made on how to treat data when an edge frame is used.

A testing project was completed to characterize the use of heat release measurement to characterize the 'non-combustibility' of products.

Reports and Publications

"North American Experiences in the Use of Cone Calorimeter Data for Classification of Products," Babrauskas, V., pp. 89-103 in *Proceedings of the International EUREFIC Seminar 1991*, Interscience Communications, London (1991).

"The Effect of Oxygen Concentration on CO and Smoke Produced by Flames," Mulholland, G., Janssens, M., Yusa, S., and Babrauskas, V., submitted to *Fire Safety Science – Proc. of the Third International Symposium* (1991).

"Standardizing the Exchange of Fire Data – The FDMS," Babrauskas, V., Peacock, R.D., Janssens, M., and Batho, N.E., *Fire and Materials. 15*, 85-92 (1991).

"Heat Release Rate: The Single Most Important Variable in Fire Hazard," Babrauskas, V., and Peacock, R.D., pp. 67-80 in Fire Safety Developments and Testing: Toxicity, Heat Release, Product Development, Combustion Corrosivity, Fire Retardant Chemicals Association, Fall 1990 meeting, FRCA, Lancaster, PA (1990).

"Effective Measurement Techniques for Heat, Smoke, and Toxic Fire Gases," Babrauskas, V., *Fire Safety J. 17*, 13-26 (1991).

"Modern Test Methods for Flammability,"Babrauskas, V., NISTIR 4326, Natl. Inst. Stan. Tech. (1990).

"Analysis of Large-Scale Fire Test Data,"Peacock, R.D., and Babrauskas, V., *Fire Safety J. 17*, 387-414 (1991).

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - 1991

FIRE HAZARD ASSESSMENT METHODOLOGY

Professional Personnel

Richard D. Peacock, Project Leader
Walter W. Jones, Group Leader, Fire Hazard Analysis Group
Glenn P. Forney, Computer Scientist
C. Lynn Forney, Mathematician
Phyllis Martin, Computer Specialist

Objective

To produce a fundamental capability to analyze the hazards associated with a specified fire scenario.

Scope

Each year, billions of dollars are spent to protect occupants and equipment against fire and fire related damage and loss. Yet in spite of the increased spending many people continue to die annually and there is still a large dollar loss. To ameliorate these problems, a systematic approach to understanding the effect of fires in buildings is necessary. The fundamental capability has been provided as a fully-supported software package for personal computers. While initially limited to residential-style occupancies, the software design is aimed at an across the board use of a broad range of applications from fire safety education to fire reconstruction.

Technical Accomplishments

BFRL developed the software HAZARD I, which predicts the hazard to a building and to occupants any where within the building. The fire hazard assessment methodology embodied in the HAZARD I software provides a vehicle which state-of-the-art fire science can be applied to improve fire safety. Continued enhancement of its capabilities and validity is a primary aspect to the mission of BFRL's fire program. Version 1.0 was released in summer of 1989. Version 1.1 was released in the fall of 1991. This latter includes new phenomenon and features to continue providing a state-of-the-art tool for hazard analysis for use by fire protection professionals. One of the new features is mechanical ventilation. We have also improved the documentation by integrating the example cases in the technical reference.

Simultaneously, work is continuing on improving the modeling capability for version 1.2. As discussed in the 1990 conference, the model now runs in extended memory under DOS, and also on Unix platforms. This will allow us to extend the fire model to more compartments. The current plan is for 20. We also support the Unix platform with X Windows, which should make the modeling more widely available.

New physical routines which have been added: flow through holes in ceilings and floors; another zone for each compartment that contains a fire. This is the ceiling jet and makes the estimate of heat loss from to the ceiling much more realistic; finally, a new radiation model is now used which solves the boundary discrepancy between convection/conduction and radiation. Besides being consistent, this

has allowed us to develop the algorithm which can be used for the self-consistent pyrolysis model.

Much of the time this year has been spent on validation of the model, that is comparing the output from the model with full scale experiments as well as fires in actual buildings. We chose five examples which push the limits of the modeling capability. This was intended to show how well the model acutally does work, and to provide guidence on what areas need to be addressed next in order to improve its capability in a significant manner. This work is discussed in one of the papers cited below. It shows excellent agreement between the two, with difficulties where we expected.

The resulting model will provide a predictive tool for manufacturers, purchasers, architects, FPE's, code officials, and practitioners to evaluate safety performance, code equivalency, and code change proposal issues.

Reports and Publications

"A Prototype Methodology for Fire Hazard Analysis", R. D. Peacock and R. W. Bukowski, Fire Technology, *26*, 15 1990.

"Analysis of Large-Scale Fire Test Data", R. D. Peacock, and V. Babrauskas, Fire Safety Journal, *17* 387, 1991.

"A Users Guide for RAPID, Version 2.3," R. D. Peacock, J. N. Breese, and C. L. Forney, NIST SP 798, October 1990.

"Data for Room Fire Model Comparisons," R. D. Peacock, S. Davis, and C. L. Forney, NIST Journal of Research, July, 1991.

"A Sensitivity Analysis of a Simple Fire Growth Model," C. L. Forney and R. D. Peacock, to be published.

Associated Grants

"Modifications to Furniture Fire Model for HAZARD System," M. A. Dietenberger, University of Dayton Research Institute.

"Mathematical Modeling of Human Egress from Fires in Residential Buildings," M. Kostreva, Clemson University.

"Incorporating Convective and Radiative Heat Transfer into the Code CCFM.VENTS," W. F. Moss, Clemson University.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 91

Institution: Clemson University

Grant No.: 60NANB0D1023

Grant Title: Mathematical Modeling of Human Egress from Fires in Residential Buildings

Principal Investigator: Michael M. Kostreva, Professor
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Clemson University
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Telephone: (803) 656-2616

Other Professional Personnel: Malgorzata Wiecek, Assistant Professor
Teodros Getachew, Doctoral Student
Mark Cawood, Doctoral Student

NIST Scientific Officer: Richard Peacock

Technical Abstract:

Research supporting mathematical modeling of egress of individual occupants from residential buildings is being performed in this project. Techniques include multiple objective analysis and dynamic programming.

To date, this research project has produced some significant findings and discovered that there are some areas that would benefit from more research. The mathematical setting for the fire egress analysis is a network superimposed on a residential building. Nodes in the network represent locations within and around the building, while links comprise potential egress routes. Each link carries one (or more) attributes, to be referred to as costs. The assignment of nodes, links and costs are made to closely reflect an actual scenario. Each occupant in the building is initially located at a unique node of the network, an origin node. The problem is to find, for each such occupant, a path of minimum cost leading from his/her origin node to a single destination node. This formulation matches one of a classical network model: the Shortest Path Problem (SPP).

The Building and Fire Research Laboratory has recently published the computer package entitled HAZARD I, which incorporates two distinct

mathematical models: FAST and EXITT. FAST is a multi-room zone fire model designed to provide a complete history (several time series, at discrete steps) of the smoke, heat and concentration of certain toxic chemicals in each room. The EXITT model accepts the output of FAST as input. Considering a group of building occupants who are specified by age, sex, and state of awakeness, EXITT applies a heuristic methodology to simulate the exit paths of these individuals by considering various decision rules. The decisions of these individuals are assumed to be taking place in the same time interval as that considered by FAST, even though the two models are run consecutively, rather than simultaneously.

In our research, solving the SPP is considered. The approach is based on Richard Bellman's Principle of Optimality: "An optimal policy has the property that whatever the initial decisions are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision". The principle gives rise to the development of a technique known as dynamic programming (DP) that has been successfully applied to solving decision problems of a sequential nature. The SPP falls in this category of decision problems due to its objective (goal) of making an optimal decision at each stage of the process, i.e. choosing an optimal link at each node of the network. DP is particularly attractive for egress analysis because it permits all the enhancements and improvements to be placed into a single mathematical framework.

Applying DP to fire egress modeling allows for generalization of the network assumptions made in the current version of EXITT and development of a unified framework for handling a new more complex model based on a multiple objective dynamic network in which links and nodes may be removed, and in which link weights are multiple and changeable in time. Such assumptions approach the network model from a perspective not previously considered in the literature. Although these features increase the mathematical complexity of the problem, the network model becomes a more realistic representation of variable environment. The network evacuation model is, in fact, strongly multiple objective in nature. There are various performance measures of a physical nature and of a behavioral nature inherent to the problem. Any meaningful model possesses dynamics due to an expanding and evolving fire and its changing parameters. Similarly, the egress path decision making should be dynamic and comprehend some 'look ahead' on the part of the evacuees.

As a working assumption in the research completed to date, it is assumed that a vector time-dependent cost function is associated with each link of the network. The vector cost always includes time as one of its components according to the intention of finding the shortest (fastest)

path in the network. The other components (objectives to be minimized) are not specified but could include distance to travel, concentration of toxic chemical on the link, density of smoke, average temperature on the link, etc. Since the multiple objectives on links are usually in conflict with each other (the fastest path need not be the shortest or the least toxic) the goal is to generate nondominated paths for each occupant, i.e. paths which are optimal in the sense that all their costs cannot be decreased simultaneously. The criteria listed above might also include personal judgement of evacuees, who are likely to behave in a multiple objective manner, namely to have multiple preferences while making a decision of choosing an optimal egress path.

The results we have obtained so far are encouraging but not complete. Some of them are contained in the paper (Kostreva, Wiecek and Getachew, 1991) which has been recently presented at the Third International Symposium of Fire Safety Science in Edinburgh, Scotland. Some will appear in (Kostreva and Wiecek 1991) which is in preparation. Initial calculations demonstrate that the methods of dynamic programming and multiple objective optimization can be successfully used to solve the following problems:

1)Finding best egress paths from all given origin nodes to a destination node, for single and multiple criteria models.

2)Finding the optimal paths when a node (representing a room or part thereof) is rendered impassable by fire or smoke.

From the point of view of results useful to reducing fire losses, one may compare such solutions over a range of fire scenarios and note the differences between fire and non-fire optimal solutions. Doing so gives a method of evaluation of the risk inherent in a building design. That is, if there is a large change, the building design is of high risk, while if there is little change, it is of low risk.

The research described here is directed toward enhancement of mathematical modeling of human egress from fires in residential buildings. Multiple objective dynamic programming has been selected as an advanced optimization technique which is capable of more faithfully representing the complex decisions being made during egress. The latest theoretical studies indicate that this approach can be generalized and applied to decision problems with time dependent cost parameters. Moreover, multiple objective dynamic programming relates very well to the mathematical models already in existence at CFR and so there is great potential for incorporating this methodology into the successors of HAZARD I.

Reports and Papers:

Kostreva, M. M., Wiecek, M. M., and Getachew, T., Optimization Models in Fire Egress Analysis for Residential Buildings, to appear in Proceedings of Fire Safety Science, Third International Symposium, International Association of Fire Safety Science, Edinburgh, Scotland, July 1991.

Kostreva, M. M. and Wiecek, M. M. , Modeling Fire Egress Paths for Residential Buildings, ICIAM 91, Second International Conference on Industrial and Applied Mathematics, Washington, DC, July 1991.

Kostreva, M. M. and Wiecek, M. M. , An Algorithm for Time Dependent Multiple Objective Path Planning with Step Function Cost Vectors, 14th International Symposium on Mathematical Programming, Amsterdam, The Netherlands, August 1991.

Kostreva, M. M., and Wiecek, M. M., Time-Dependency in Multiple Objective Dynamic Programming, in preparation,1991.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution: University of Dayton Research Institute

Grant No.: 60NANB0D1051

Grant Title: Modifications to Furniture Fire Model for HAZARD System

Principal Investigator: Mark A. Dietenberger
Associate Research Physicist
University of Dayton Research Institute
300 College Park - JPC/232
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(513) 229-3037

Professional Personnel: David Grove, Research Programmer

NIST Scientific Officer: Dr. Walter W. Jones

Technical Abstract:

Introduction. This grant supported the modifications to the furniture fire model (FFM) for eventual inclusion in the HAZARD system. Three major tasks were performed: (1) the FAST/FFM predictions were compared with several full scale burns measured in the furniture calorimeter, (2) an algorithm for the calibration of the ignition and flame spread parameters for PC application was developed and coded, and (3) assistance was provided to successfully convert FFM to a Flame Spread Model (FSM) for a single panel. The code was implemented on the PC for use with CFAST. These developments should find applications in fire scenarios relating to compartmentation, structural fire resistance, ignitibility of a secondary combustible item, and room flashover. Further details can be found in reports and papers being published.

Model Validation With Data. The FAST/FFM (Version 3) predictions were compared with a set of full scale fire tests listed in NBS Monograph 173, "Fire Behavior of Upholstered Furniture," by Babrauskas and Krasny. The full scale database contained the furniture calorimeter measurements of heat and mass release rates, the soot extinction areas versus time, and the VCR recordings of flame spreading on each cushion panel versus time. The corresponding bench-scale database from the cone calorimeter and the flame spread apparatus at various irradiance levels of very similar materials was essential. These existing bench-scale and full-scale fire databases were acquired from NIST and tabulated. In particular, six different fabric/foam combinations were chosen and the model scaling constants were calibrated for each one.

The scaling constants associated with the heat and mass

release rates were calibrated on similar materials tested with 3 or 4 different values of the cone heater radiances. This calibration was a two step procedure. The first step was to calibrate a constant surface heat flux, which adjusts the calculated net surface heat flux, in order to rescale the heat and mass release data for different radiances onto a single curve as a function of burn history. Further details are in Reference 1. The second step was to adjust the burn history parameters in order to convert from a 50 mm thick foam used in the cone calorimeter to a 100 mm thick foam used in the upholstered furniture.

The soot parameters of maximum absorption coefficient and specific extinction area were assumed to be that for the polyurethane foam. The current cone calorimeter measurements of the soot extinction area and the soot mass fraction as a function of time can be converted to the maximum absorption coefficient and the specific extinction area as a function of burn history. Using the conventional approach, the surface ignition temperature and the thermal thickness were derived from the piloted time to ignition data versus irradiance. Since in all furniture fire tests the piloted ignition was located on the seat middle and 100 mm from the back rest, the constant for the flame spread rate was calibrated to obtain agreement with the observed burn area fraction of the seat. When this data was not available, the flame spreading constant was calibrated to match the timing of the rapid rise in the heat release rate.

The excellent comparisons of the cushions burn area fraction between FFM and the data in Figure 1 demonstrate the model's unique ability to accelerate the flame spread rate due to the fire's rising thermal radiation. The good comparisons of the heat release rate between the model and the data in Figure 2 for the 5 different furniture geometries were achieved using a single set of model constants. The results also demonstrate that the rapid flame spread up the back rest accentuates the flame spreading on the seat due to the increased plume radiation. The peak heat release rate, shortly after the rapid flame spreading, shows its dependence on the total burning area as well as on the magnitude of the thermal radiative heat fluxes from the fire plume. Further results with the remaining fabric/foam materials and with different mockup constructions are in a paper being prepared.

Ignition And Flame Spread Parameters. The calibration of the ignition and flame spread parameters in opposed flow involve two steps: (1) a scheme to determine material constants, such as ignition temperature, thermal inertia, and thermal thickness, from the piloted ignition measurements, and (2) a scheme to obtain the flame spread constants from the LIFT and from a horizontal flame spread apparatus. It is assumed that these apparatus are designed such that there is negligible thermal radiation from the fire plume to the flame front. This allows a direct evaluation of the flame spread constants apart from the indirect use of FFM (and FSM). As a result, the algebraic formulations of the flame spread rate could be used in the curve-fitting algorithms developed and coded for use

on the PC.

In order to understand the effects of the flame spread directions on the flame spread constants, it was necessary to extend the classical deRis formulae to account for the effects of surface thermal radiation, changing gas properties, the Damkohler's number, and the buoyant air flow. At present, only the PMMA has been measured in enough flame spread configurations to derive some relevant conclusions. Most opposed-flow flame spread experiments were done in the downward direction, giving the lowest flame spread rate.

The fit to the LIFT data of time to ignition versus irradiance for the clear PMMA provided a thermal inertia of 0.5 $(kW/m^{2o}K)^2s$ and an ignition temperature of 645 ^oK. The curve fit of the modified deRis formulae to the downward flame spread as a function of time is shown in Fig. 3. The corresponding constants are the flame sheet temperature of 1327 ^oK and a buoyant velocity of 230 mm/s. These values are consistent with results obtained with other experiments in which the varied parameters include oxygen mass fraction, pressure, tangential gravity, forced opposed flow, and imposed irradiances. Those results are reported in a paper being prepared. Here, we only report the fitted values for downward, lateral, and horizontal flame spread. For lateral spread on the LIFT, the fitted values are, T_f = 1485 ^oK and V_g = 328 mm/s.

For the black PMMA, the fit to the data for horizontal flame spread as shown in Figure 4, correspond to T_f = 1563 ^oK, and V_g = 389 mm/s. This is in agreement with Dipert's measured value of T_f = 1560 ^oK in the flame sheet and to 1320 ^oK in the flame foot. It appears the flame temperature and the induced airspeed increases in progression with downward, lateral, and horizontal flame spread. All the values seem reasonable. Although FFM could have been extended to fit the full data range in Figure 4, the purpose was to see how far one can go in neglecting the flame radiance. The constants above can be converted to the flame foot heat flux and length used as inputs to FFM. The FFM can then be used to determine how negligible the flame plume radiance was on the flame spread rate, as assumed above.

FSM Development. The FFM was simplified and made more user friendly by downsizing to a Flame Spread Model (FSM) for a single panel. We assisted the FHA group in this conversion. The computer memory requirements were significantly reduced and the inputs to FSM were documented better. The several simulations of a wall fire spread has revealed certain anomalies, which were corrected by improving the flame spread logic and by restricting the panel geometry to avoid large errors in the view factor evaluations. The results with FSM are described in more detail in a different project summary and will be published as a NIST technical report.

References.

1. M. A. Dietenberger,"Technical Reference and User's Guide For FAST/FFM Version 3," NIST-GCR-91-589,1991.

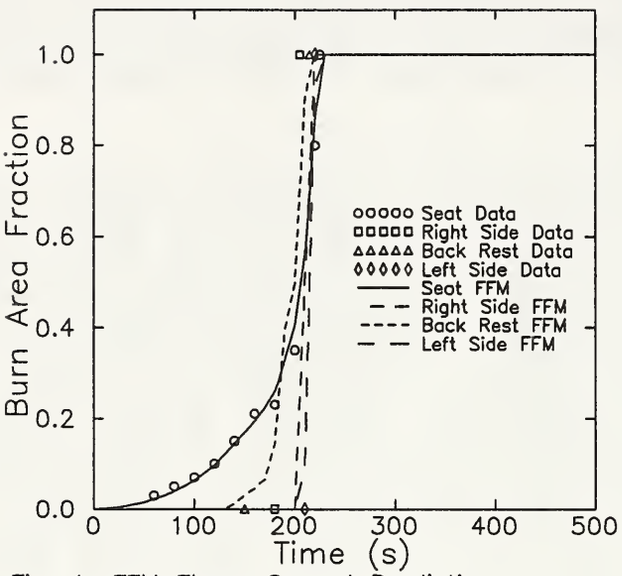


Fig. 1. FFM Flame Spread Prediction And Comparison With Data For FR Foam/HO Fabric, 4–Cushion Chair

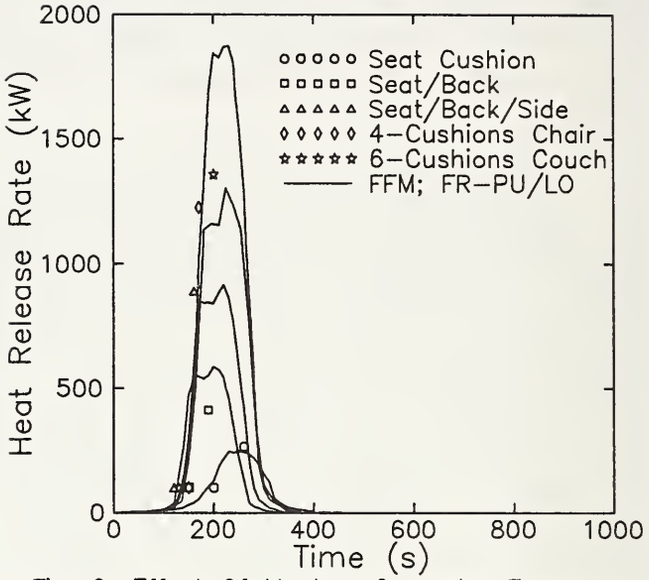


Fig. 2. Effect Of Mockup Geometry For 100 mm, FR Foam/LO Fabric Cushions And Comparisons With Data

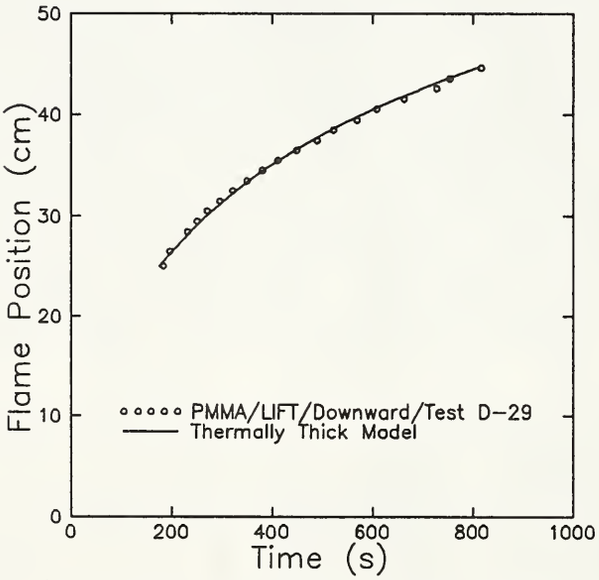


Fig. 3. Flame Spread Curve Fit Versus LIFT Data in Downward Flame Spread Assuming Zero Flame Radiance

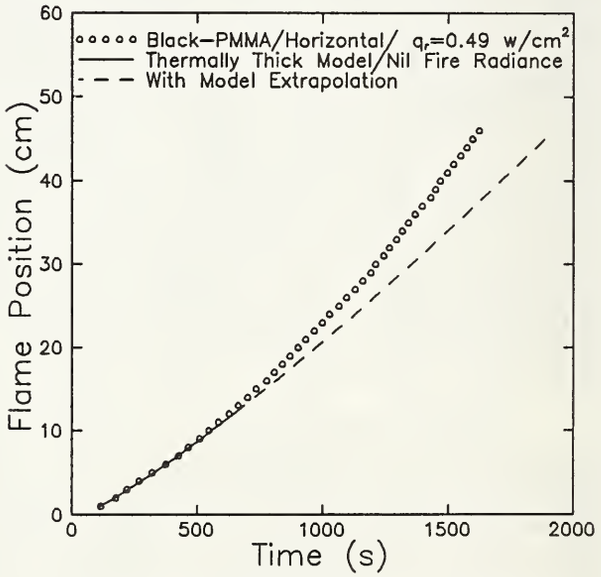


Fig. 4. Flame Spread Curve Fit Versus Data (Dipert's) on Horizontal Surface Assuming Zero Flame Radiance

1.10 Engineering Analysis Systems

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - 1991

ENGINEERING METHODS

Professional Personnel

Harold E. Nelson, Project Leader
C. Arnold, Computer Programmer

Project Objective

1. The development of separated and assembled fire protection analytical (computerized) tools and the transfer of these tools to practicing professionals.

2. The use of these tools and other resources to recreate and otherwise analyze one or more significant fires. To initiate verification of the results, to evaluate the tools, and to assist decision makers in actions to prevent recurrence.

Scope

1. Assemble useful data, formulas, and simple models. Program these into a common format with an accessible point of entry (menu, etc.) Develop this into a generalized engineering approach suitable for compartmented buildings. (This portion of the project is closely allied with aspects of the GSA sponsored Engineered Fire Protection Assessment System project.)

2. Demonstrate procedures for fire reconstruction investigations. Conduct a reconstruction investigation of one or more fires of significance. Analyze the fire, determine and initiate research or testing needs required for a satisfactory reconstruction, prepare the appropriate report.

Technical Accomplishments

1. Engineering Analysis System.

FPETOOL, a computerized package of simple, easy to use, engineering equations and models has been issued and widely distributed. The program has been upgraded in format and presentation. Updates and improvements continue. Underway are procedures to estimate the gravity wave front that can occur in a corridor following flashover and the flow of smoke from a hazard laden corridor into an area of refuge. A training manual has been developed for the General Services Administration (GSA) and two training courses conducted.

2. Fire Reconstruction.

Two fire reconstruction efforts were undertaken. The more interesting is the analysis of the fire in the Hillhaven nursing home in Norfolk, VA. In that fire tests of representative bed systems were tested in both a free burn and room configuration. The burning in the ASTM room flashed over generating more than a two fold increase in heat release rate as compared to the freeburn test. (See

Figure 1). The increased burning level appears to be a result of the rapid burning of the paper facing on the gypsum board lining used in the ASTM room during this test. The investigation and analysis also indicated that a gravity wave front containing lethal concentrations of carbon monoxide likely flowed from the fire room in this incident through the corridor, then passed through doors that were slightly ajar into the bedrooms of the victims.

Funding from Other Agencies/Institutions

In addition to BFRL Priority Project funding the above activities were carried out with significant support from GSA and the Department of Health and Human Services.

Reports and Publications

"FPETOOL: Fire Protection Engineering Tools for Hazard Estimation," Harold E. Nelson, NISTIR 4380.

"FPETOOL User's Guide," Harold E. Nelson, NISTIR 4439.

"Comparing Compartment Fires with Compartment Fire Models," Harold E. Nelson and Scott P. Deal, presented at 3rd International Symposium for Fire Safety Science, Edinburgh, Scotland, 1991.

"History of Fire Technology," Harold E. Nelson, presented at the Conference on Firesafety Design in the 21st Century, Worcester Polytechnic Institute, Worcester, MA, 1991.

"Engineering Analysis of the Fire Development in the Hillhaven Nursing Home Fire, October 5, 1989," Harold E. Nelson, NISTIR 4665.

Related Grants

"Fire Safety in Board and Care Homes," Carl M. Harris, George Mason University.

CENTER FOR FIRE RESEARCH
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY 91

Institution: George Mason University

Grant No.: 60NANB9D0974

Grant Title: Fire Safety in Board and Care Homes

Principal Investigator: Prof. Carl M. Harris, Chairman
Dept. of Operations Research & Applied Statistics
George Mason University
4400 University Drive
Fairfax, VA 22030-4444

Other Professional Personnel: Dr. Bernard M. Levin
Dr. Norman E. Groner
Roseanne Paulsen

NIST Scientific Officer: Harold E. Nelson

Technical Abstract:

Project Objectives

The goal of this project is to collect, analyze, and disseminate technical information that will help lead to a high degree of fire safety in board and care homes without incurring unnecessary expense or interfering with program goals. This information will be related, in large part, to the use of the Board and Care Chapter of the 1985 and 1988 editions of the Life Safety Code.

This grant involves several independent tasks, each contributing to the goal of the project.

Progress and Problems in Adoption of the Board and Care Chapter of the Life Safety Code

A major emphasis of this project is to determine the extent to which the Board and Care Chapter of the National Fire Protection Association's Life Safety Code has been adopted, and to uncover problems with its use and interpretation. Such knowledge can be helpful in developing recommendations for refinements of the Code and in promoting its use.

During the first year of the project, information was obtained from state officials, mostly from social service agencies, with knowledge of how the chapter is being applied in their state. During this second year of the project, information was sought from two additional groups -- inspectors for the Veterans Administration and "board and care" home providers. Responses were entered into a computer database using Paradox software. Analyses of the data, including essay type responses, were completed.

Veterans inspectors survey. With input from the project staff, the Department of Veterans Affairs surveyed their employees in the field who do the board and care fire inspections as part of the DVA Community Residential Care

Program. The responses were made available to the project staff. The DVA refers veterans only to those board and care facilities which meet the requirements of the Board and Care Chapters of the Life Safety Code. While the tenor of the comments from the 106 respondents was generally favorable toward the Board and Care Chapter (Chapter 21) of the 1988 Code, the respondents did discuss a wide range of problems related to its use. Problems most frequently encountered by providers, as stated by these inspectors, included the costs of fire safety features (particularly those incurred in retrofitting older homes), the use of certain hardware features such as door closers, and the complexity of dealing with more than one set of applicable regulations. With respect to the inspectors' own experience in using Chapter 21 to evaluate community facilities, the response was about evenly split between those who thought Chapter 21 was not difficult for them to apply and between those who thought Chapter 21 was somewhat difficult to use. A specific objection was to the complexity generated by Chapter 21's references to provisions in other chapters of the Life Safety Code. Also, it was pointed out that some inspectors were responsible for only a few board and care homes: the DVA inspectors had ample opportunity to forget the details of the code between annual inspections.

Provider survey. The George Mason project staff mailed requests for information to 974 providers of different types and sizes of facilities distributed thoughout the country about their attitudes and experiences with fire safety regulations. George Mason received 219 meaningful responses plus an additional 16 responses from a pilot study. (Five respondents provided more than one usable response, i.e., information on two facilities that were significantly different from each other.) To date, one or more responses have been received from 44 states. Although many more small facilities responded, the response from the larger facilities represented a much greater number of residents. Responses were overwhelmingly from facilities which are either licensed or certified or both. About 10 percent of the letters sent were returned as undeliverable, or the respondent indicated that the facility had gone out of business: this would tend to indicate that there is a large turnover in the provision of board and care services.

Most providers responded to the question, "In your personal opinion, is the level of fire safety protection required too low, about right, or too stringent?", with the answer "about right" (91% of the 224 respondents to date who chose to answer this question). An analysis of the comments of the respondents who answered "**about right**" shows that several of them felt that the regulations were somewhat too strict in some specific areas. (None of those who answered "about right" specifically expressed concern about the regulations being too lenient, although a few indicated they had done more than their regulations required, i.e., installed sprinkler systems.) Areas, where regulations seemed too strict to some of this group of respondents, were exit sign requirements, fire drill frequency, heavy doors, and automatic door closures. Exit signs were regarded as institutional looking and perhaps unnecessary in smaller residential facilities; too frequent fire drills were thought to lead to resident complacency and lack of response; and heavy doors and automatic door closers were regarded as somewhat of a hazard to residents. Many elderly and/or depressed residents do not like having their doors shut and will keep them propped open. Some respondents volunteered their view that "small" homes are not very different from regular family homes and should, therefore, not be treated differently from regular homes. We conclude that most providers accept the need for the fire safety requirements and do not wish major changes; however, some of these providers would like to see some specific changes, and these are in the direction of more leniency.

Providers were asked to comment on any problems with enforcement of fire safety regulations for their facilities. Of the 230 respondents in our sample, 106 of them chose to respond to this item. Of those responding, 56% indicated that they had no problems with enforcement, while 44% indicated some degree of dissatisfaction with the enforcement system. Three respondents described situations where an enforcement problem was very significant from their point of view, as for example, costly renovations ($17,000 for a 32 bed facility) that were later determined to be unnecessary. The problem most commonly cited was differing interpretations of the regulations by different inspectors. Variations on this exist. There can be different interpretations of the rules from different inspectors from a given agency, or even from the same inspector, from one time to another. There can be inconsistency between inspectors from two separate jurisdictions presumably applying the same code, e.g., the fire marshal and a licensing agency. (Some "inconsistency" may be only perceived -- for example, a provider may not have been aware that a different edition of a code had become applicable between inspections.) Another source of frustration and perceived inconsistency stems from the fact that different social agencies or political units (city, county, state, and/or Federal government), all having jurisdiction, may be applying different sets of regulations. Several respondents cited both the different interpretations problem and the overlapping jurisdictions problems. Two respondents volunteered that health agency employees did not appear to be adequately trained as compared to building officials or fire marshals.

Brochures

Dr. Groner of the project staff has designed two attractive, easy to understand brochures that describe and promote the fires safety requirements of the Board and Care Chapter of the Life Safety Code. They emphasize the unusually varied nature of the board and care occupancy, both with regard to resident type and building type, and the flexible approach which the Life Safety Code takes to accommodate this variety. One of these brochures is especially designed to help make regulatory officials more sensitive to the goals and problems of the providers and, conversely, to make providers more sensitive to the goals and perspective of the regulators. Drafts of these brochures were reviewed by NFPA, and changes were made in response to their suggestions. The latest versions have been sent for review to all sponsoring agencies of this project.

Providers' Manual

A manual is being developed that could be used by those providers that are not knowledgeable about fire safety codes and regulations. Such providers must eventually rely on the advice of experts. However, they need a manual that will give them a simple explanation of the requirements in the Board and Care Chapter and advice on how they should proceed in preparing their facilities to meet the requirements in the Chapter. The manual should help them understand the type of professional assistance they will need. The writing of this manual is now underway.

EXITT Simulation Model

EXITT is a computer program that simulates the decisions and actions of occupants of a residence in a fire emergency. Development of a preliminary version of this model was completed before this project. The emphasis during its initial development was to demonstrate that such a model could be developed.

This emphasis was continued during the first year of this project when the model was expanded to permit staff to re-enter the building to perform additional rescues. (This new feature was necessary for the model to be used to study the fire safety of Board and Care Homes.) Dr. Harris is now investigating the sensitivity of the model to changes in parameter values. This is basic to improving the validity of the model and to making the model "probabilistic."

It is relatively easy to investigate the sensitivity of the parameters by varying each parameter independently. However, we are interested in investigating the interactions among the parameters by varying a number of parameters at the same time. This could easily lead to a number of computer runs well beyond our capabilities to run on the computer or to analyze in depth. A sampling plan is needed. We were unable to find a sampling procedure that could be easily adapted for our purpose. Dr. Harris and two of his colleagues developed a new sampling procedure that would better meet our needs. They have prepared Report No. GMU/5-26048/101, as listed below. Dr. Harris' contribution was partially supported by the grant.

Reports:

C.M. Harris, K. Hoffman, and L.A. Yarrow, "Obtaining Minimal Correlation Latin Hypercube Sampling Plans," Report No. GMU/5-26048/101, George Mason University, 1991.

B.M. Levin, "Board and Care Fire Safety Project, Interim Report," September 30, 1990.

BUILDING AND FOR FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - 1991

FIELD MODELING FOR BUILDING FIRE PHYSICS

Professional Personnel

John Klote, Mechanical Engineer, Project Leader
Glenn Forney, Computer Scientist
William Davis, Physicist

Project Objective

Develop field modeling capability at BFRL including a demonstration application of simulating transport of fire gases including detailed fluid dynamic and heat transfer effects by field modeling.

Scope

Field modeling is capable of simulating fluid dynamic and heat transfer details important to fire development and smoke transport. This level of detail is beyond the capability of other types of models. It is anticipated that this new capability will be incorporated in the projects of many BFRL groups in the future.

Technical Accomplishments

The commercial field modeling software, FLOW3D, has been acquired, and the staff have been trained in the field model software and related pre and post processing software. Features of the model were exercised including steady flow, unsteady flow, non-uniform grid, heat conduction, and graphic output. A model of a thermal link was added to the field model, and the boundary conditions were modified specifically for fire simulations.

Field model simulations were made for a one room fire experiment which included thermal links. Other simulations were made for a three room fire experiment. The results of these simulations were in good agreement with experimental data.

The field model was used as a tool for solution of a wind problem with fire fighter trainers belonging to the U.S. Navy. The field model successfully simulated flame conditions during wind conditions, and was used to develop various methods to correct the problem.

Reports and Publications

"Field Modeling of Room Fires," William D. Davis, Glenn P. Forney, John H. Klote, National Institute of Standards and Technology, NISTIR 4673.

1.11 Large Fires

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
PRIORITY PROJECT - 1991

KUWAIT OIL WELL FIRES

Professional Staff: David D. Evans, Project Leader
Daniel Madrzykowski, Mechanical Engineer
George W. Mulholland, Research Chemist
Nelson P. Bryner, Chemical Engineer

Project Objective:

Provide fire source term data for use in assessing the impact of the Kuwait oil well fires.

Scope:

Determine the heat release rate, and combustion products from burning crude oil jet and pool fires in Kuwait using ground based measurements techniques.

Technical Accomplishment:

In May 1991, a NIST research team completed two days of field survey and oil well fire measurements in the Al Maqwa Oil Field, 30 km south of Kuwait City. This effort was the first phase of a four phase effort to characterize the fire sources in Kuwait being coordinated through the World Meteorological Organization (WMO) and World Health Organization (WHO). During this Phase I effort, a number of measurements techniques to quantify the dimensions, power, and radiative characteristics of the fires were examined. Grab samples of combustion products were also collected for analysis. The Phase I effort provided the necessary experience to determine the measurement equipment and logistics needs for an extensive and longer term Phase II effort planned for the fall of 1991 to measure fire characteristics in each of the fields now burning.

Preliminary analysis of the measurements and samples collected in the Phase I effort has been completed. The Phase I report contains information on flame heights of several well fires measured from the ground and from a helicopter. Detailed thermal radiation emission from one unobstructed 56 meter tall, 1.7 gigawatt vertical jet flame are also reported. The Phase I effort showed that an extensive, systematic survey of the oil well fires is feasible and would provide a unique data base of oil fire characteristics. This information of immediate use to scientists performing an assessment of the impact of the fires, is useful in the analyzing the design of passive and active radiation exposure protection systems as well as the design of fire suppression systems for oil drilling and production facilities. The Phase I report contains a summary of the particulate and chemical analysis of the smoke grab samples collected from one of the fires. Details of these emissions measurements and analysis are contained in a separate Report of Test.

For the past 10 years, the Fire Research Program at NIST has studied the burning characteristics and suppression of petroleum fires. A long term project to understand the dynamics of jet flames associated with oil and gas well blowout fires including both burning characteristics and effects of water on the radiation and extinction of the flame has been conducted under supported from the Minerals Management Service, part of the Department of the Interior. Results of that research have shown that gas well fires can be extinguished with water sprays, radiation from oil and gas mixtures burning in a vertical jet can be predicted and the lifting and blow-off of turbulent flame could be correlated. The burning of oil spills at sea has been studied to determine the burning characteristics of the spill and the particulate and chemical emissions under support from the Minerals Management Service, U.S. Coast Guard and the American Petroleum Institute. This study has shown that burning is a means to remove rapidly large quantities of oil from the water surface and has quantified the emissions from the burning. A large scale test series involving measurements of 15 m x 15 m crude oil pan fires was completed in June, 1991 as part of this research program.

Publications :

"Preliminary Source Term Characterization of the Kuwait Oil Well Fires," D. Madrzykowski, D. D. Evans, G. W. Mulholland, H. R. Baum, B. A. Benner, R. A. Fletcher, E. Steel, S. A. Wise, W. E. May, and G. Haynes, NISTIR series report in preparation, (1991)

"Analysis of Smoke Samples from Oil Well Fires in Kuwait," G. W. Mulholland, B. A. Benner, R. A. Fletcher, E. Steel, S. A. Wise, W. E. May, D. Madrzykowski, and D. D. Evans, NIST Report of Test FR 3985, (June 20, 1991).

Related Grants:

"Computer Simulation of the Rise, Dispersion and Ground Deposition of Large-Scale Smoke Plumes," Ahmed F. Ghoniem, Massachusetts Institute of Technology.

"A Study of Simulated Oil Well Blowout Fires," Jay Gore, University of Maryland.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution: Massachusetts Institute of Technology

Grant No.: 60NANB0D1036

Grant Title: Computer Simulation of the Rise, Dispersion and Ground Deposition of Large-Scale Smoke Plumes

Principal Invesigator: Professor Ahmed F. Ghoniem
Department of Mechanical Engineering
#3-339, M.I.T
Cambridge, MA 02139

Other Professional Personnel: Xiaoming Zheng, Ph.D. Student

NIST Scientific Officer: Dr. Howard R. Baum

Technical Abstract:

Massive fires resulting from the burning of oil spills, uncontrolled oil wells, forest fires, and large-scale explosions produce large smoke plumes which rise several hundred meters before they become buoyantly stable due to entrainment and atmospheric stratification. After reaching their maximum altitude, plumes may continue to flow horizontally, oscillate around a horizontal line (cooling phase), or descend in the wind direction. The trajectories of these plumes, which determine their impact on the local, and possibly global environment, are governed by the interaction between the wind pattern, atmospheric turbulence, atmospheric stratification, ground terrain, and smoke plume properties. The purpose of this work is to develop an efficient and accurate computational simulation model for the prediction of the smoke plume trajectory, cross section and smoke distribution as the plume settles on the ground as a function of all the parameters mentioned above. The computational model is designed to run on an engineering workstation and to produce data required for assessing the impact of fires on the environment.

We have embarked on a study of plume dynamics for the purpose of developing a computer simulation model which can be used to predict trajectories of plumes arising from massive smoky fires. The purpose of the model is to provide a tool for estimating the impact of such fires on their immediate and near-field environment in terms of the induced wind velocities, smoke dispersion and its ground distribution. The intention is to have the model act as a risk assessment tool in cases when fires may be used in an oil spill clean-up and as a predictive tool for uncontrolled fires. To endow the model with a high level of universality and flexibility, it is based on a reduction of the three-dimensional Navier-Stokes equations which describe the motion of an incompressible inviscid flow in a gravitational field into their parabolized form using the wind direction as the primary flow direction. The equations are then solved numerically using a grid-free Lagrangian method which is based on the extension of the vortex method to variable density flow. The equation are then normalized to determine the independent parameters of the problem.

In a homogeneous field, these are found to be: $\varepsilon = \frac{\dot{m}_p}{\rho_o U A}$; where $\dot{m}_p$ is the smoke mass flow rate, ρ_o is the atmospheric density, U is the wind speed and A is the plume cross-sectional area; and the initial height, HT, and shape, R_y/R_z, of the plume cross section.

During the past year, we focused on (1) optimizing the simulation code by determining the range of the numerical parameters within which the simulation is accurate and economical; (2) investigating the effect of initial height and shape on the plume trajectory and smoke distribution on the ground; and (3) formulating an extended model of plume motion in wind-sheared and density-startified atmosphere. We also performed a preliminary study on plume interactions.

Figure 1 shows results of a typical simulation in terms of a smoke concentration contour and a vorticity contour. The plume cross section is an ellipse with an aspect ratio of three and its initial height is five times its minor radius. The plume shape is modified substantially as it falls. During the initial stages, vorticity is formed within the zone of finite density gradient between the plume material and the atmosphere. Next, the vorticity rolls up into two large counter-rotating eddies, which form at the far ends of the plume cross section, causing a substantial deformation of the plume cross section into a 'horseshoe' U-shape. Strong entrainment currents are set by the eddies and a portion of the plume kinetic energy is lost to the surrounding air leading to a slow down in its downward motion. As the plume approaches the ground, its cross section experiences substantial flattening and its material spreads over a width which grows well beyond its original major axis. While the plume is settling, some of the smoke is ejected upwards due to the action of the large vortices and their images. Clearly, the area within which the smoke of the plume disperses is much larger than its initial cross section and depends strongly on the local conditions and the plume properties. The smoke distribution near the ground is far form Gaussian and is more closely described by a uniform distribution with two peaks on the sides.

The goal of this work is to produce a simulation code which can be run efficiently, in response to anticipated or existing fire senarios, on an advanced engineering workstation Thus, it is important to minimize the run time without sacrificing the accuracy. For this purpose, we performed an extensive computational study to determine the effect of each numerical parameter on the accuracy and computer time requirements. The goals were to prove that as each numerical parameter is refined one can reach convergence, and to find the largest value of each numerical parameter which maintains accuracy. It was found that the most critical parameters are the distance between neighboring elements, the core radius of each element and the time step (distance along the wind direction). In most cases, the numerical simulations reproduced the large-scale features accurately within a wide range of each parameter. For a typical case, $O(100)$ elements are sufficient to discretize the plume cross section at $t = 0$. As the simulation proceeds and the plume cross section becomes more convoluted, the adaptive nature of the computational scheme allows the addition of more elements to accurately capture these changes. We found that for most cases, and until $\varepsilon < 1.0$, the Boussinesq approximation is adequate for providing the required accuracy.

The effect of the initial plume height was invesigated by fixing its cross section, as a $3x1$ ellipse, and changing its height between 3-30. Figure 2 shows the change in the mass average vertical drop, measured as the distance between the initial location and the current location, and the width of the plume. The initial stages of all cases; during which a vortex layer forms and rolls up into a horseshoe, are similar. During these stages, the plume acceleration is almost constant, i.e $H_p \approx x^2$. As the plume falls further, a series of secondary roll-ups on the lower side of the plume are observed. This further contributes to the redistribution of the plume material in the horizontal direction and the generation of turbulence near the ground. As the plume settle on the ground, its width increases at a faster rate and an upwards ejection of some of its material is observed. The ground effect becomes important around $H_p \approx 2$. The total circulation of each eddy increases at a constant rate until the plume approaches the ground when this rate drops quickly. We found that each eddy can be described as a monopole which becomes a dipole as the small scales are entrained into the horseshoe. Analytical models are being developed to summarize these results.

The shape of the initial plume cross section is found to have an important effect on its trajectory. Figure 3 shows the mass average vertical drop and the normalized plume width for different shapes. Plumes with compact, i.e. circular cross sections fall faster than those with extended cross sections flattened in the horizontal direction. They entrain more and their dispersion in the horizontal and vertical directions occurs faster. We find that all these features are due to a faster rate of vorticity generation in the plume with a circular cross section. Thus, while plumes with circular cross sections reach the ground earlier, their smoke is expected to spread over a smaller area than that of an elliptical plume.

We are currently analyzing results of multiple plume interactions and the effect of atmospheric stratification on plume dynamics.

Papers and Reports:

Ghoniem, A.F., Zhang, X.M., Knio, O.M., Baum, H.R. and Rehm, R.G., "Numerical simulation of the dynamics of negatively buoyant plumes," to be submitted for publication at Physics of Fluids.

Zhang, X.M., Knio, O.M. and Ghoniem, "A Lagrangian vortex method for thermals and plumes," to be submitted for publication at the Journal of Computational Physics.

Zhang, X.M., and Ghoniem, A.F., "Entrainment, settlement and multiple interactions in falling plumes," to be submitted for publication at Atmospheric Environment.

Ghoniem, A.F., Computer Simulation of the Rise, Dispersion and Ground Deposition of Large-Scale Smoke Plumes, First Annual Report, in preparation.

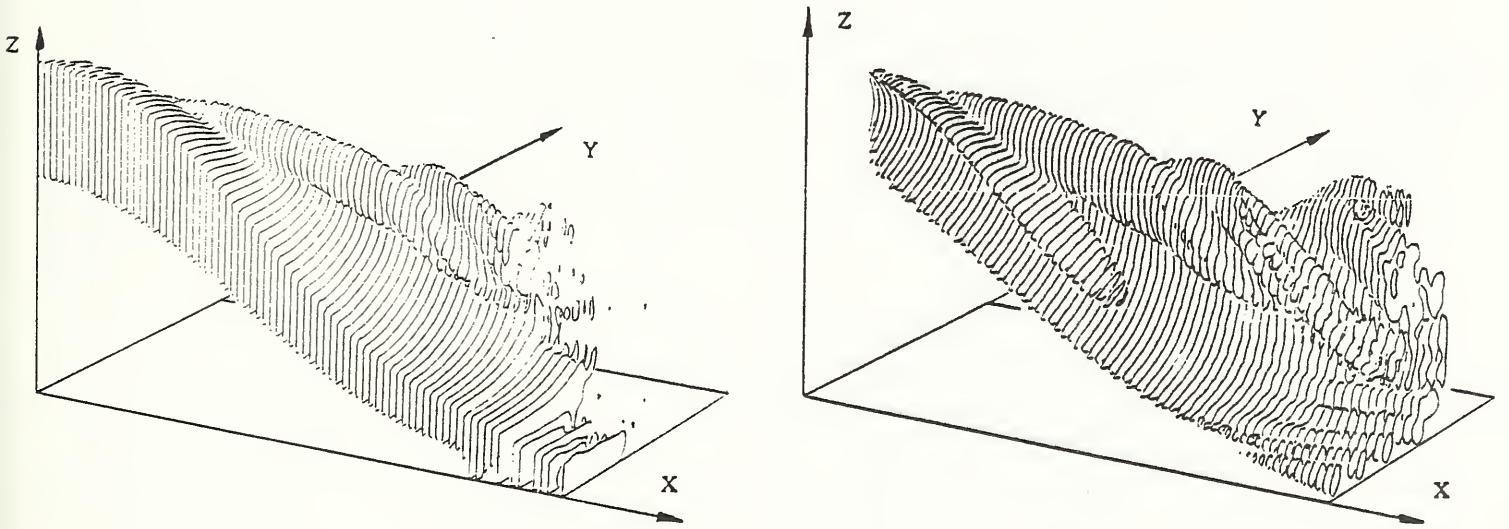
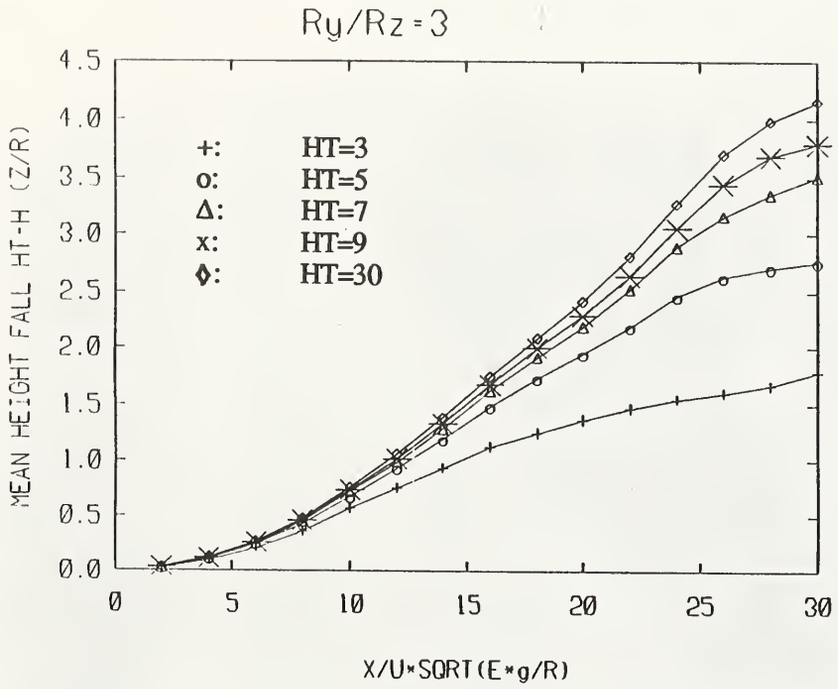


Figure 1. Three dimensional plots showing surfaces of smoke constant density (left) and constant vorticity (right) in the descending plume. The plume starts at a height equal to five times the minor axis of its elliptical cross section. The major axis is three times the minor axis. For $\varepsilon = 0.1$, the ratio of the plume density to the air density is 1.0106. The density surface contour value is 1.003 and the nondimensional vorticity surface contour value is 0.2.



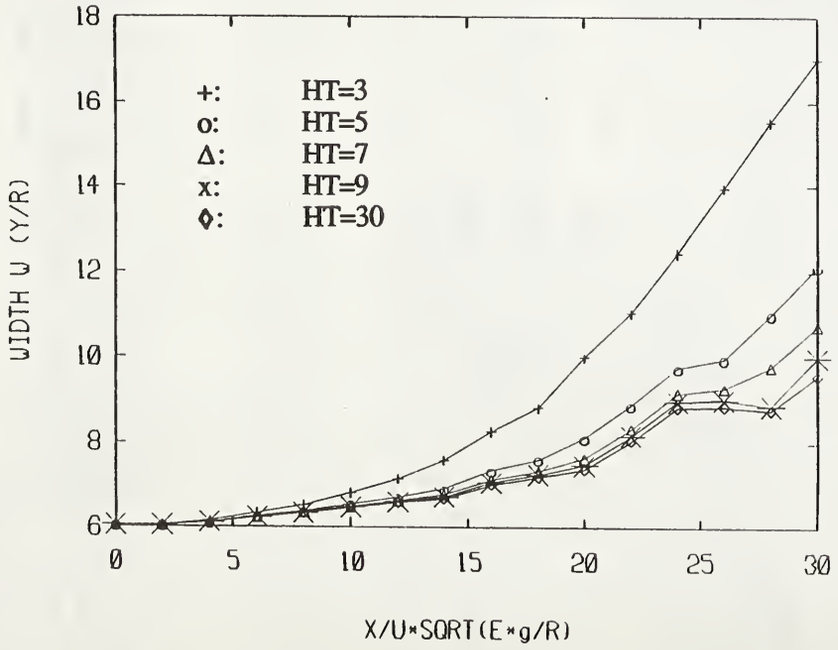
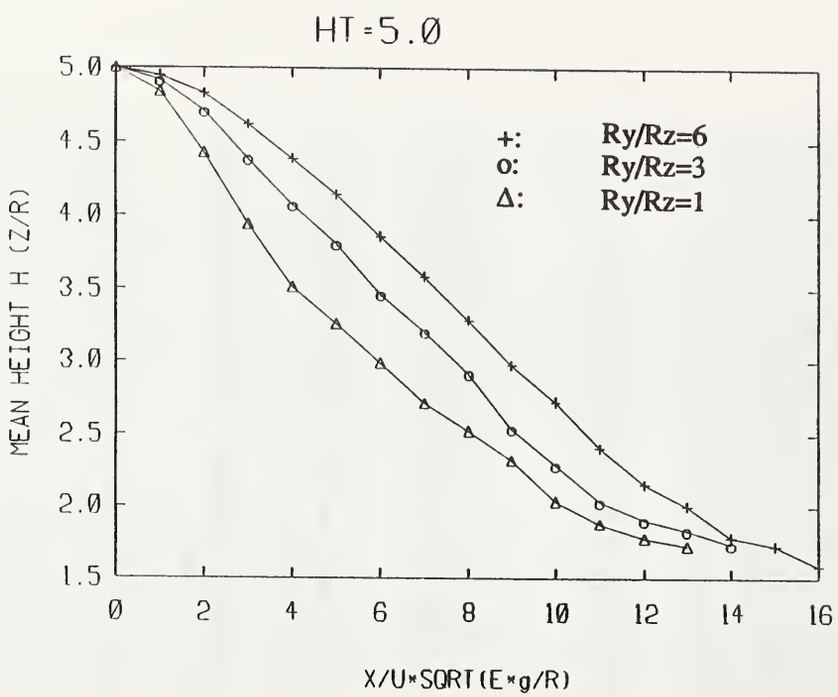


Figure 2. Mean height fall (top) and width (bottom) of plumes with the same initial cross section, Ry/Rz=3, and different initial heights, HT=3 - 30.



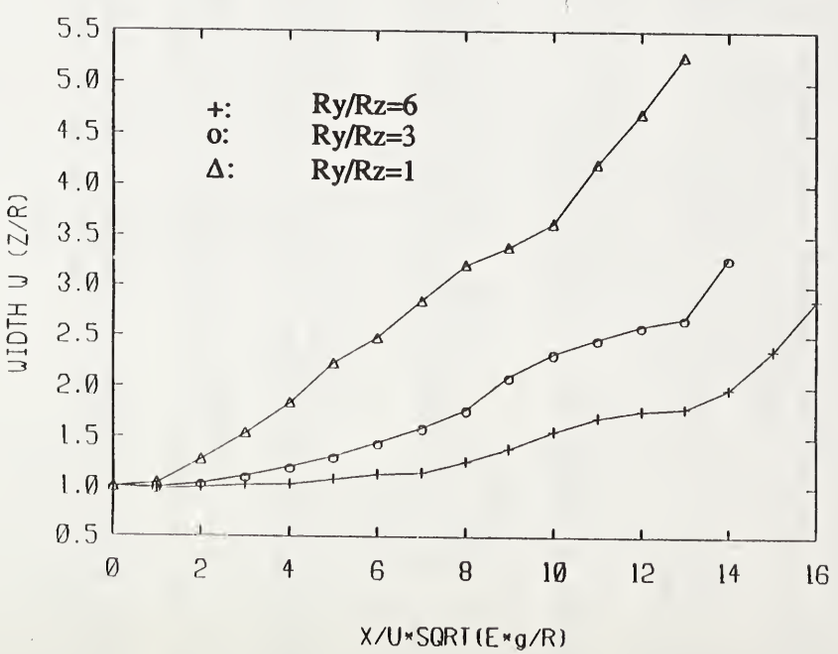


Figure 3. Mean height (top) and width (bottom) of plumes with the same initial height, HT=5, and different initial cross sections, Ry/Rz=1 - 6.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution: University of Maryland

Grant No: 60NANB8D0834

Grant Title: A Study of Simulated Oil Well Blowout Fires

Principal Investigator: Dr. J. P. Gore
Mechanical Engineering Department
University of Maryland
College Park, MD 20742

Other Personnel: Dr. Y. Sivathanu, Research Associate
Mr. C. Q. Jian, Doctoral Student
Mr. S. M. Skinner, Graduate Student

NIST Scientific Officer: Dr. David D. Evans

Technical Abstract:

Introduction: The overall objective of this program is to develop technology for obtaining engineering predictions of radiation hazard to personnel and structures resulting from oil and gas well-blowout and diverter fires as well as accidental fires and flares on offshore platforms. Effect of water suppression on the radiation heat fluxes is also of interest. During the past year, three problems related to radiation loads resulting from oil and gas well fires were addressed : (1) state relationships for fuel mixtures, (2) the effects of buoyancy turbulence interactions, and (3) phenomena related to two phase jet fires.

(1) State Relationships for Fuel Mixtures: Mixing rules for state relationships for major gas species in flames burning fuel mixtures (all oil and gas fires involve fuel mixtures) have been developed and verified experimentally. Measurements of concentrations of major gas species burning mixtures of CH_4 and C_2H_2 in air have been completed. The results are interpreted in terms of the laminar flamelet concept. For fuels with minimal sooting tendency, the mixture rules and the generalized state relationships provide identical estimates of the major gaseous species. However, the mixture rules provide much better estimates of CO_2, CO and H_2O in mixtures involving sooty fuels.

(2) Buoyancy Turbulence Interactions: Horizontal jet flames are common in accidental pipe leaks, diverter fires and flares on offshore platforms. Flames in the horizontal configuration have been studied sparsely compared to their vertical counterparts.

The global characteristics of horizontal jet flames known

previously involve a progressive turn away from the horizontal due to buoyancy forces, a shorter visible flame length (L_f) even in the curvilinear coordinate system following the turn, and a larger flame width along the trajectory. In the present study, it was discovered that for the range of exit conditions considered, the flow-field involves multiple transient plumes of hot gases on the upper interface of the curvilinear horizontal jet. This unique flow field is expected to affect the mixing, combustion and radiation characteristics of the flames in the horizontal configuration.

Measurements completed thus far include: (1) mean and fluctuating velocities in three directions using a laser Doppler velocimeter (LDV); (2) video flame photography and image analysis for studying the mean and RMS flame length, flame width and intermittency of the visible flame interface; (3) mean species concentrations of CO_2, CO and unburnt hydrocarbons using a water - cooled stainless steel sampling probe and online infrared analyzers; (4) mean temperature distributions in the flames using fine wire thermocouples; and (5) total radiative heat fluxes on semi-infinite surfaces entirely surrounding the flames using a wide angle radiometer. All measurements were performed for three horizontal flames burning methane in air and their vertical counterparts with identical burner conditions.

As a first step, a two dimensional numerical analysis involving a low speed parabolic axisymmetric jet flow in an adaptive curvilinear coordinate system was used in conjunction with the laminar flamelet hypothesis and a buoyancy modified mixing length model of turbulent mixing to predict the trajectories and distributions of velocity, temperature and gas species in the jet flames. Vertical counterparts of the flames were also treated using the model as a baseline.

Figure 1 shows measurements and predictions of flame trajectories of three horizontal flames stabilized at the exit of a 6 mm diameter long stainless steel tube burner. The analysis provides encouraging estimates of the flame trajectories for a range of exit Reynolds numbers. It is noted that integral analyses reported in the literature recently do not agree with the experimental measurements shown in Fig. 1 and underestimate the overall horizontal spread of the flames considerably.

Figure 2 shows measurements and predictions of velocities in the curvilinear coordinate direction (S) plotted as a function of normalized distance from the flame axis. Results for three locations involving positions where the visible flame has turned only slightly (S/L_f =0.25), where the visible flame is in the process of making a rapid turn (S/L_f= 0.5) and finally at location where the turn is almost complete (S/L_f =0.75) are shown. As seen from Fig. 2, the predictions match the measurements in the jet region of the flow-field but entirely miss the plume flow. A 2.5D numerical code is currently being developed to address these non-symmetric effects.

Measurements of radiative heat fluxes for horizontal flames showed that the radiative heat loss fractions X_R for these flames are consistently higher (by a factor of 1.2) than their vertical counterparts. This observation is of interest from practical considerations as well as for understanding the fundamentals of flame radiation properties.

(3) Two Phase Jet Fires: Three jet flames involving Alberta sweet crude oil atomized by methane at heat release rates of 34, 29 and 19 kW were studied. Measurements involved flame photography and radiative heat loss fractions. The 34 kW fire involved predominantly crude oil (2 kW from the atomizing methane), the 29 kW fire involved a 15 kW methane fire and the 19 kW fire involved a 5 kW methane flame. Surprisingly, the radiative heat loss fractions for all three fires were in the range 20 % +-3 %.

Differences in atomization quality, combustion efficiency and temperatures are believed to be responsible for this behavior. Further study of these fires is in progress.

Acknowledgement: The continued support from MMS is appreciated.

Reports and Papers:

1. J. P. Gore, D. D. Evans and B. J. McCaffrey, "Temperature and Radiation of Diffusion Flames with Suppression," Combust. Sci. Tech., Vol. 77, pp. 189-202, 1991.
2. J. P. Gore and S. M. Skinner, "Mixing Rules for State Relationships of Methane and Acetylene/Air Flames," Comb. Flame, in press, 1991.
3. J. P. Gore, U. S. Ip and Y. R. Sivathanu, "Coupled Structure and Radiation Analysis of Acetylene/Air Flames," ASME J. Heat Trans., revised, 1991.
4. J. P. Gore and C. Q. Jian, "A Study of Trajectories of Horizontal Buoyant Turbulent Jet Flames," ASME J. Heat Transf., submitted, 1991.
5. J. P. Gore and C. Q. Jian, "Comments on Scaling of Buoyant Turbulent Jet Diffusion Flames by N. Peters and J. Gottgens," Comb. Flame, submitted, 1991.
6. J. P. Gore and C. Q. Jian, "Flame Trajectories of Buoyant Horizontal Jet Flames," Proceedings of the ASME/JSME Thermal Engineering Conference 1991, Vol. 5, pp. 127-138, 1991.
7. S. M. Skinner and J. P. Gore, "State Relationships for Acetylene + Methane/Air Flames," Proceedings of the Twenty-Third Fall Technical Meeting of the Eastern States Section of the Combustion Institute, Orlando, FL, pp. 58.1-58.4, 1990.
8. J. P. Gore and S. M. Skinner, " A Study of Simulated Oil Well Blowout Fires-Part 1," University of Maryland Report, College Park, MD, 1990.
9. J. P. Gore and C. Q. Jian, "A Study of Simulated Oil Well Blowout Fires-Part 2," University of Maryland Report, College Park, MD, 1990.
10. S. M. Skinner, " A Study of Mixing Rules for Scalar State Relationships for Fuel Mixtures," Master of Science Thesis, Department of Mechanical Engineering, The University of Maryland, College Park, MD, 1990.

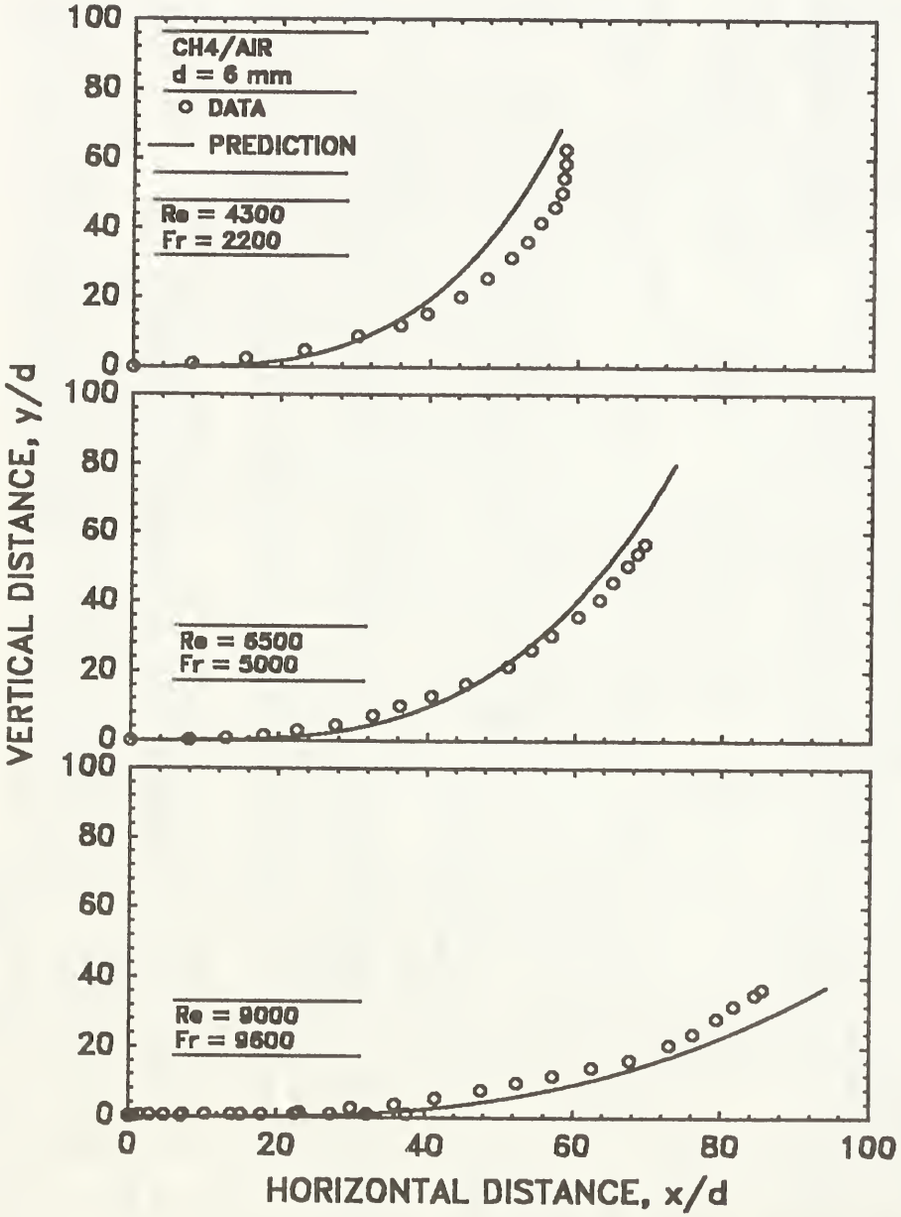


Fig. 1 Measurements and Predictions of Trajectories of Horizontal Jet Flames

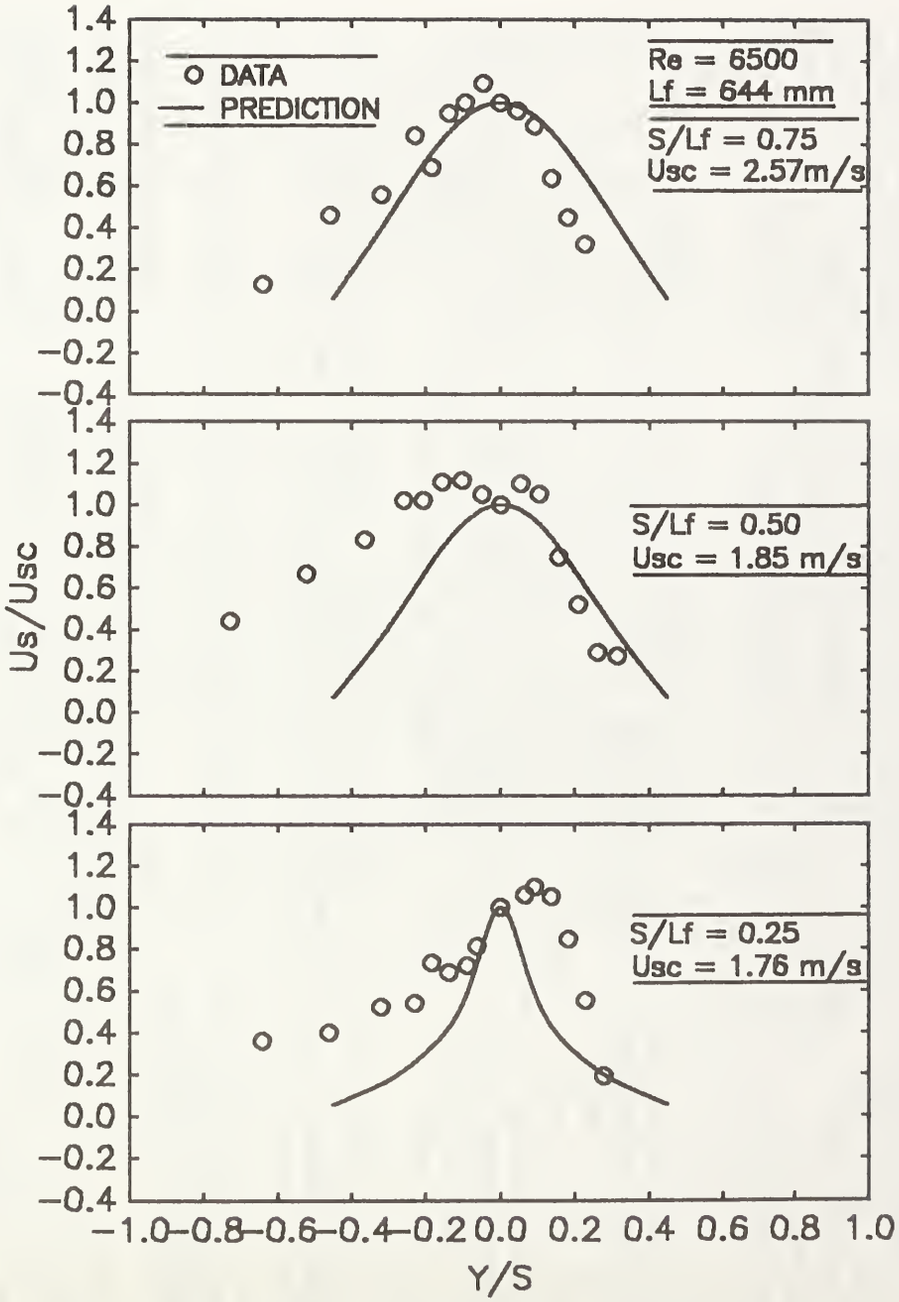


Fig. 2 Measurements and Predictions of Velocity Distributions

2.0 Timely Response to Current Fire Problems (mostly projects funded by other agencies of private sector organizations)

2.1 Fire/Modeling Interactions

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

ALGORITHM DEVELOPMENT FOR CFAST

Funding Agency

Nuclear Regulatory Commission

Professional Personnel

Walter W. Jones, Project Leader
Leonard Y. Cooper, Mechanical Engineer
Glenn P. Forney, Computer Scientist
Richard D. Peacock, Chemical Engineer
Richard W. Bukowski, Electrical Engineer

Technical Accomplishments

Traditionally, a zone model calculates heat loss from the upper layer to a boundary surface simply by using a heat transfer coefficient and the difference in temperature between the adjacent gas layer and the boundary surface. This presumes complete mixing of the gases, a normal assumption for a zone model. However, in the case of a fire plume, the gases in the plume generally have not completely mixed with the upper layer. Thus, this gas will in general be at a higher temperature than the gas in the upper layer, and consequently the heat transfer to the ceiling will be greater. Further, the actual temperature and velocity profiles will be affected by the placement of the plume within the compartment. To include these effects in CFAST, a ceiling jet model was incorporated. It was done so as to allow for the plume being placed off the centrum of the compartment. The latter was done so that the heat transfer to the ceiling is dependent on the relative position of the fire plume in the compartment. This was instantiated by integrating the velocity profile over a rectangular area from an arbitrary point on the surface of the ceiling. With the fire placed away from the centrum of the room, the ceiling jet will not spread symmetrically away from the fire, thus modifying the actual heat loss rate, and subsequently the time to activation of a sprinkler link. Several numerical simulations were done to ascertain the effect on gases exiting a compartment of the placement of the fire within a room.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

CIGARETTE IGNITION METROLOGY

Funding Agency: U.S. Consumer Product Safety Commission

Professional Staff:
Richard G. Gann, Project Leader
Emil Braun
Richard H. Harris, Jr.
Henri Mitler
Thomas J. Ohlemiller
Kay M. Villa
George N. Walton

Project Objective:

Fulfill NIST responsibilities under P.L. 101-352, the Fire-Safe Cigarette Act of 1990, by August 9, 1993. The Act directs NIST to perform three tasks for the CPSC: develop a standard test method to determine cigarette ignition propensity, compile performance data for current cigarettes using the method, and conduct laboratory studies on and computer modeling of ignition physics to develop a predictive capability.

Technical Accomplishments:

BFRL has developed approaches to both primary (direct measurement of ignition) and secondary (measurement of another property related to ignition propensity) test methods. These will be tested using the experimental cigarettes that were supplied by the tobacco industry during the Cigarette Safety Act of 1984. Measurements have been made on ignition and substrate temperature distribution as a function of oxygen level, weight of substrate fabric, padding, and applied heat flux from a cigarette-simulating source. These data are to guide the test method and the modeling. A computer model of a substrate degrading in the presence of a moving heat source has been developed, eventually to run in conjunction with one of a cigarette burning on a non-reactive substrate. The former solves the time-dependent heat diffusion equation and includes an asymmetric, variable size, moving computational grid; two pyrolyzing layers with an air gap in between; and temperature-varying thermophysical properties.

Reports and Publications:

"The Effect of Cigarette Characteristics on the Ignition of Soft Furnishings," Gann, R.G., Harris, R.H., Krasny, J.F., Levine, R.S., Mitler, H.E., and Ohlemiller, T.J., NBS Technical Note 1241, National Institute of Standards and Technology, Gaithersburg, MD, 1988.

"Reevaluation of Experimental Cigarettes used in the Cigarette Safety Act of 1984," Harris, Jr., R.H., Navarro, M., Gann, R.G., and Eberhardt, K.R., NIST Report of Test FR 3984, National Institute of Standards and Technology, Gaithersburg, MD, 1991.

"Global Kinetic Constants for Thermal Oxidative Degradation of a Cellulosic Paper," Kashiwagi, T. and Nanbu, H., submitted to Combustion and Flame, 1991.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991
COPPER INTERACTIONS WITH FIRE GASES

Funding Agencies: International Copper Association, Ltd.
The Society of the Plastics Industry, Inc.

Professional Staff: Barbara C. Levin, Project Leader
Emil Braun, Physicist
Richard H. Harris, Jr., Chemist
Magdalena Navarro, Biologist
Maya Paabo, Consultant, Research Chemist

Project objectives:

1. To determine if the reduced levels of HCN generation and resultant toxicity from copper-impregnated flexible polyurethane foams previously observed under small-scale conditions in our laboratory still occurs under large-scale conditions.

2. To examine the effects of reduced oxygen conditions on the toxicant suppressant capability of cuprous oxide when impregnated in flexible polyurethane foams.

Technical Accomplishments:
Previous reports from this laboratory have shown that flexible polyurethane foams (FPU) treated with copper dust, cupric oxide, cuprous oxide or copper sulfate produced significantly less (90%) hydrogen cyanide (HCN) when thermally decomposed than the identical but untreated control foams. The decreased atmospheric concentrations of HCN resulted in the reduction of the acute inhalation toxicity (as measured by lethality in Fischer 344 rats) produced from exposure to this smoke. This reduction of HCN and toxicity occurred regardless of whether the copper or copper compound was added to the foam during its formulation (prior to the foaming process) or added as a post-treatment (after formulation). In all these reported experiments, the foams were thermally decomposed in the cup furnace smoke toxicity apparatus via a two phase procedure previously shown to produce high concentrations of HCN. Last year the following flammability properties were examined in foams with and without 0.1% cuprous oxide: 1. ignitability in three systems 2. rate of heat release, 3. smoke obscuration, and 4. rate of flame spread. In all cases, no differences in flammability characteristics between the treated and untreated foam were observed. Full-scale (room burns) tests of chairs composed of copper-impregnated (1%) foam cushions are currently being conducted to examine the effect of different combustion conditions. Initial results look promising.

Reports and Publications:
A New Approach for Reducing the Toxicity of the Combustion Products from Flexible Polyurethane Foam, Levin, B.C., Paabo, M., Braun, E., and Harris, R.H., Jr., Proceedings of the 2nd Annual BCC Conference on Flame Retardancy "Advances in Flame Retardancy of Polymeric Materials, Stamford, CT, May 14-16, 1991.

Reduction of Hydrogen Cyanide Concentrations and Acute Inhalation Toxicity from Flexible Polyurethane Foam Combustion Products by the Addition of Copper Compounds; Part III. The Effect of Copper Additives on the Flammability Characteristics of Flexible Polyurethane Foam, Levin, B.C., Braun, E., Shields, J.R., and Lowe, D., NISTIR 4441, National Institutes of Standards and Technology, Gaithersburg, MD, 1990.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

FIRE AND SMOKE SPREAD IN SHIPS

Funding Agency

Naval Research Laboratory

Professional Personnel

Walter W. Jones, Project Leader
Paul A. Reneke, Computer Scientist
Emil Braun, Physicist

Objective

To provide data analysis, predictive capability, display and data acquisition in support of full scale fire testing on the ex USS SHADWELL.

Technical Accomplishments

The CFAST model and associated support programs were installed on the ex USS SHADWELL in FY 1990. During FY 1991, the most recent version of CFAST was installed on the Navy computer systems based on the ex USS SHADWELL. This includes mechanical ventilation, hydrogen chloride deposition, vertical flow and display of the results. Included in the model is the capability for calculating vitiated combustion, rocket fuels and class A materials. As part of the validation and verification process, the data obtained in full scale test on the SHADWELL was analyzed and compared with the CFAST model. A derivative module specific to Navy applications was developed to read and display sensor information in real time.

Reports and Publications

"Comparison of Full Scale Fire Tests and a Computer Fire Model of Several Smoke Ejection Experiments," E. Braun, D. L. Lowe, W. W. Jones, P. Tatem, R. Carey and J. Bailey, NISTIR 1991.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

FLAME RETARDANT STUDY

Funding Agency: General Electric Co.

Professional Staff: Takashi Kashiwagi, Project Leader

Project Objective:

To understand the effects of polymer structure and certain flame retardant treatments on flammability properties of GE's engineering thermoplastics.

Technical Accomplishment:

Various flammability properties, ignition, flame spread rate, heat release rate, CO and soot yields, and smoke extinction, are measured for various GE's polycarbonates, polyimides and polyphenyleneoxides with and without flame retardant treatments. The effects of external radiant flux on the flammability properties of these sample were determined using Cone Calorimeter and LIFT devices. Since all of these samples intumesce during burning, two sample mounting configurations are used. One of them is with a metal frame and a course grid to retain the sample surface at the original location. The other is without any frame or a grid and the sample intumesces without any restriction. The former tends to generate lower heat release rate and the latter higher heat release rate. Since the sample size used in the Cone Calorimeter is relatively small (about 10 cm x 10 cm), the amount of intumescent might be affected by the size. In order to study this effect samples with the size of 38 cm x 38 cm will be tested to measure the amount of intumescent and also heat release rate.

Gasification rate, temperature distribution in the sample, and evolved gaseous products of selected combinations of polymer samples will be measured using the new radiative gasification device. The gasification experiment will be conducted in nitrogen atmosphere to make certain that there are no gas phase reactions. The sample will be exposed to external flux up to 75 KW/m^2. Samples with and without the treatments will be studied to determine the effects of the treatments on the gasification process and hopefully to understand the mechanism of the flame retardant treatment.

Reports and Publication:

"Effects of Sample Mounting on Flammability Properties of Intumescent Polymers", Kashiwagi, T. and Cleary, T.G., submitted to Fire Safety J.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

MATERIAL FLAMMABILITY TEST ASSESSMENT

Funding Agency: NASA

Professional Staff: T. Ohlemiller, Project Leader
K. Villa, Textile Technologist
J. Shields, Physical Scientist

Project Objective:

Assess the current NASA flammability test method against the set of tests currently in use at NIST for measuring the elements of material flammability.
Assess the role of radiative self-feedback in flammability enhancement.

Technical Accomplishments:

A set of materials was tested using the standard NASA flammability assessment method (NHB 8060.1B) in ambient air and using the ignition, rate of heat release and lateral flame spread tests developed at NIST. The NASA test looks at the tendency for upward flame spread on a small sample of a material when subjected to a small flaming ignition source for a fixed duration (approx. 25 sec). Only one of the tested materials exhibited substantial upward flame spread in this test; the others exhibited minimal upward spread. The NIST tests all subject a material to a range of incident radiant heat fluxes comparable to those expected from the burning of other objects near the object of interest. Under these circumstances, given a sufficient external flux (which varies with the nature of the material), all of the materials ignite, exhibit a significant rate of heat release and lateral flame spread rate. The NASA test was modified to permit radiative pre-heating of the sample and sample holder to facilitate flame spread. The response of the materials to this pre-heating varied widely. One required little external flux to yield full upward spread while others showed little response to the maximum absorbed flux. An attempt was made to predict this varied response using flammability data obtained in the NIST tests and a simplified analytical model of upward spread due to Quintiere and Cleary. The model predictions did not correlate well with the modified NASA test results; the reasons seem to lie in limitations both in the model and in the input data. Some of the issues raised are still being pursued.

The second objective above will be addressed experimentally. The radiative view factor directly affects the extent of self-feedback between elements of a burning surface. This factor will be varied by changing the area initially ignited in a configuration that mimics two parallel burning surfaces on a single material; a mirror will be substituted for the second surface to achieve nearly equivalent radiative feedback to the actual burning surface. The minimum feedback flux that facilitates flame spread will be examined, first for downward spread and then upward spread. The latter should correspond to levels found in the modified NASA test.

Publication:

"Material Flammability Test Assessment for Space Station Freedom", T. Ohlemiller and K. Villa, NISTIR 4591, June, 1991

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1992

RADIATIVE IGNITION AND SUBSEQUENT FLAME SPREADING IN MICROGRAVITY ENVIRONMENT

Funding Agency: NASA Microgravity Science Program

Professional Staff: Takashi Kashiwagi, Co-Project Leader
Howard R. Baum, Co-Project Leader
Hiroshi Yamashita, Guest Researcher
Kazuyoshi Nakabe, Guest Researcher

Project Objective:
Develop a theoretical model to be able to predict ignition and subsequent flame spreading over a thin cellulosic material in a microgravity environment using the material characteristics determined in normal gravity.

Technical Accomplishment:
Two-dimensional, two-dimensional axisymmetric, and three-dimensional time-dependent ignition and subsequent flame spread with slow forced flows from 0 to 10 cm/s in microgravity has been developed. Its gas phase model is based on irrotational flow mainly controlled by the slow forced flow, gas expansion and mass addition from a degrading condensed fuel with one-step oxidative reaction with energy and chemical species equations. Its condensed phase model is based on the thermally thin cellulosic sheet with three global degradation reactions, pyrolysis reaction and oxidative degradation of the sheet to generate char and gaseous products, and oxidative char degradation. Preliminary results show that ignition parameters, the size of irradiated area, its duration and flux, have significant effects on transition to flame spread. The effects of flow velocity, oxygen concentration, the size and its duration of external radiant flux, with and without a pilot, and many other parameters (gas phase reaction kinetics,..) on transition from ignition and flame spread will be studied. It appears that transition from spontaneous ignition to flame spread tends to be difficult without the slow flows. Determination of kinetic constants of the three degradation reactions was completed using TGA analysis with multiple heating rates and oxygen concentrations and by continuous evolved gas analysis of CO, CO_2, H_2O and O_2. The development of an apparatus to measure global gas phase oxidation reaction rates for the degradation products from the cellulosic sheet will begin shortly.

Reports and Publication:

"Heat and Mass Transport From Thermally Degrading Thin Cellulosic Materials in a Microgravity Environment", Kushida, G., Baum, H.R., Kashiwagi, T. and Di Blasi, C., accepted publication in J. Heat Transfer.

"Global Kinetic Constants for Thermal Oxidative Degradation of a Cellulosic Paper", Kashiwagi, T. and Nambu, H., submitted in Combustion and Flame.

"Heat and Mass Transport From Heated Material in a Low Reynolds Number Microgravity Environment", Yamashita, H., Baum, H.R. and Kashiwagi, T., to be presented at Fourth International Conference on Numerical Combustion sponsored by SIAM, December 1991.

2.2 Fire Protection Technology

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

COMPARTMENT FIRE MODEL TO SIMULATE THE EFFECTS OF ROOF VENTS, SPRINKLERS, AND THEIR INTERACTIONS

Funding Agency: AAMA Research Foundation

Professional Personnel: Leonard Y. Cooper, Project Leader
William Davis, Physicist

Program Objectives

Development of a computer fire model for engineering analysis of roof vents, sprinklers and their interactions during fire-generated environments.

Technical Accomplishments

The generic fire scenario to be analyzed is depicted in Figure 1. The analysis and the corresponding computer code must capable of simulating smoke layer growth in a curtained area of a building space. The action of fusible-link-actuated ceiling vents on the fire environment is taken into account. The model also takes account of first sprinkler actuation by a fused link and the effect of subsequent sprinkler-spray cooling of the accumulating ceiling-level smoke layer on subsequent sprinkler link responses. The fire is assumed to be specified. The goal is to predict the effects of various vent deployment and actuation schemes within the sprinkler-operating environment.

The work of developing the computer model has been divided into two major stages. Each stage involves the formulation of mathematical algorithms for

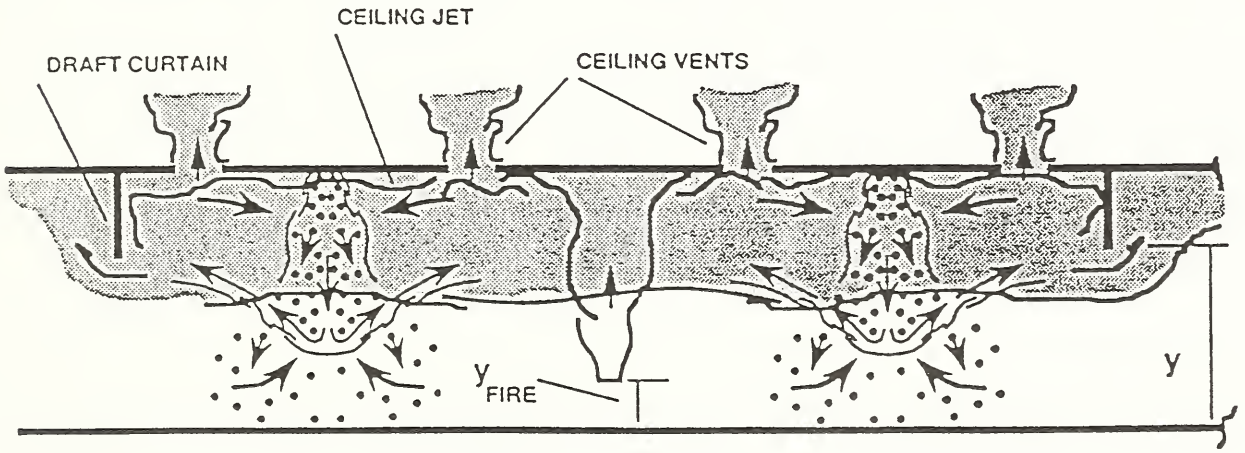


Figure 1. Fire in a building with draft curtains and fusible-link-actuated ceiling vents and sprinklers.

particular aspects of the problem, the development of their solution in terms of computer code, and the demonstration of the computer code to yield sound and consistent results over a range of parameters.

Stage 1: The effect of roof venting on the actuation of sprinkler links.

Stage 2: Stage 1 with the added effect of sprinkler spray discharge.

Work on Stage 1 was completed in previous years. This resulted in the user-friendly computer code LAVENT (Link-Actuated VENTs) and a comprehensive User Guide (NISTIR 89-4122). This code implements the model equations developed and presented in [1]. LAVENT simulates the fire environment and the response of arbitrarily deployed fusible-links, as depicted in Figure 1, up to the time of actuation of the first sprinkler. An overview of LAVENT is presented in [2]. Reference [3] describes a parametric study of fusible-link actuation which was carried out with LAVENT. The Stage-2 effort, completed this year, resulted in a prototype of an advanced version of LAVENT, called LAVENTS (Link-Actuated VENTs and Sprinklers), which includes a modular subroutine for simulating the interaction of an isolated sprinkler and an upper layer of arbitrary temperature and thickness. The details of the interaction model, which extends and generalizes ideas in [4], are presented in [5].

Reports and Publications

Cooper, L.Y., Estimating the Environment and the Response of Sprinkler Links in Compartment Fires with Draft Curtains and Fusible Link-Actuated Ceiling Vents - Theory, Fire Safety Journal 16 (1990) pp. 137-163.

Davis, W.D. and Cooper, L.Y., A Computer Model for Estimating the Response of Sprinkler Links to Compartment Fires with Draft Curtains and Fusible-Link-Actuated Ceiling Vents, Fire Technology, Vol. 27, No. 2, pp. 112-127, May 1991.

Davis, W.D. and Cooper, L.Y., A Study of Fusible Link Actuation Using a Two Dimensional Ceiling Jet Model, LAVENT, (in review) to be submitted for outside publication.

Heskestad, G., Sprinkler/Hot Layer Interaction, Factory Mutual Research Corporation Report to NIST, NIST-GCR-91-590, National Institute of Standards and Technology, Gaithersburg MD, May 1991.

Cooper, L.Y., Interaction of An Isolated Sprinkler Spray and a Two-Layer Compartment Fire Environment, NISTIR 4587, National Institute of Standards and Technology, Gaithersburg MD, May 1991.

Related Grants

Flow Through Horizontal Vents as Related to Compartment Fire Environments, Jaluria, Y., Rutgers - The State University of New Jersey.

Sprinkler/ Hot Layer Interaction, Heskestad, G. Factory Mutual Research Corporation.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution: Rutgers, The State University of New Jersey
New Brunswick, New Jersey

Grant No.: 60NANB7D0743

Grant Title: Flow Through Horizontal Vents as Related to Compartment Fire Environments

Principal Investigator: Professor Yogesh Jaluria
Department of Mechanical and Aerospace Engineering
Rutgers, The State University of New Jersey
New Brunswick, NJ 08903
Telephone: (908)932-3652

Other Professional Personnel: A. Abib (Ph.D. Student)
Q. Tan (M.S. Student)
T. Fan (Research Assistant)

NIST Scientific Officer: Dr. Leonard Y. Cooper

Technical Abstract:

Introduction This investigation was initiated in September 1989 in order to experimentally study the flow rate across a horizontal vent in an enclosure with non-zero pressure and density differences imposed across the vent. The flow through such vents, which may be ceiling or floor vents in a multi-room compartment, is important in the mathematical modeling of the fire growth and smoke spread in the compartment. The removal of the combustion products from the room and the inflow of oxygen to sustain the fire are both dependent on this flow across the vent. The fluid below the vent is generally lighter than that above it because of the temperature difference. Also the pressure within the enclosure rises due to the fire. As a consequence, a pressure difference Δp results across the vent and tends to force the fluid from within the enclosure to the outside or to the connecting compartment. The density difference $\Delta\rho$, on the other hand, tends to force fluid, particularly oxygen, into the room across the vent, due to density being higher on the outside. In addition to Δp and $\Delta\rho$, the thickness to diameter ratio of the vent L/D arises as a parameter. This work is directed at understanding the basic transport processes that arise and govern the flow across the vent and at determining the resulting flow rates, correlating these in terms of the governing parameters. The results are expected to be of particular interest to vented room fires and the flow rates obtained would be provided as inputs to the mathematical modeling of these fires.

Experimental System A fresh-water/salt-water flow arrangement has been used to simulate the density difference that arises across the vent due to a fire in the

compartment. This system allows density difference ratio $\Delta\rho/\bar{\rho}$, where $\bar{\rho}$ is the mean density, up to around 0.2, which corresponds to the value for a temperature difference of 100K in gases at an average temperature of 500K. The pressure difference Δp is imposed by moving, up or down, a storage tank for fresh water connected to the bottom of the main tank, which is 0.74 m long, 0.44 m wide and 0.62 m high, with a horizontal partition at 0.31 m from the bottom, see Fig. 1. The vent or vent tube is at the center of this partition plate. The pressure differences of interest are very small, generally being in the range 10-100 N/m^2. These pressure differences are easily obtained with this arrangement. The resulting pressure difference across the partition plate is measured in the quiescent environment far from the flow region by means of a small pressure differential transducer made by Omega, with a full scale pressure differential of around 250 N/m^2. The flow rate across the vent is obtained by measuring the density variation in the upper region with time and the flow rate of fresh water entering the compartment from the side. The stopper is removed for a specified time interval, the two regions are well mixed after the vent is closed and the density of the fluid in the upper region is measured, using hydrometers. Several hydrometers, covering different density ranges, are employed to accurately measure the density resulting from the mass transfer across the vent over the given time period. A shadowgraph is used for flow visualization, indicating when the flow is uni- or bidirectional. A hot-film anemometer is employed to measure the velocity level in the region close to the vent. Both circular and rectangular vents are used, with a wide range of height to diameter, or width, ratio L/D. Several results have been obtained during the course of this study. Some of the typical results are presented and discussed in the next section.

Experimental Results At zero pressure difference, which is obtained by closing the valve at the side entrance to the tank, a bidirectional flow arises across the vent, with the volumetric upflow equal to the downflow (Epstein, J. Heat Transfer, 110, 885, 1988). The shadowgraph indicated the basic trends, with the upper heavier fluid descending in the central region of the vent and the lighter lower fluid rising in the outer region. Density measurements were taken over wide ranges of $\Delta\rho$ and L/D. From these results, the flow rates were determined. The results obtained are shown in Fig. 2 in terms of the dimensionless flow rate, or Froude number, as a function of L/D. Clearly, the results are well correlated in terms of these variables, over the parametric ranges investigated. Also, there is good agreement between the present results and the earlier work, lending strong support to the accuracy of the experimental results.

The shadowgraph was also used to investigate the decrease in the downward flow rate as the pressure difference Δp is increased. This flow rate was found to decrease to zero, followed by a unidirectional upward flow as the pressure difference is increased further. The flow rate was found to increase as the imposed pressure difference is increased. Therefore, the observed physical behavior was very much as expected and indicated the switch from a bidirectional to a unidirectional flow as the pressure difference was increased. The hot-film anemometer indicated similar trends in terms of the velocity level being monitored just above the vent at the center. Some of the photographs from the shadowgraph have been presented in Refs. (1,2) given below.

The main emphasis of this study being on the flow under a nonzero pressure difference, most of the effort over the last year has been directed at the purging, or flooding, pressure difference at which the downward flow due to the density difference is stopped

by the imposed pressure and at the flow rates arising for nonzero pressure and density differences for both uni- and bidirectional transport across the vent. Some of the typical results are presented in Figs. 3 and 4. Figure 3 shows the measured variation of the upper region density ρ_u with time for different vents. As expected, it was found that the upward flow increases with increasing pressure difference and decreases with an increase in the opposing density effect. With L/D, the trends are more involved due to different flow regimes that arise, as seen in Fig. 2 for zero pressure difference. The purging pressure was studied as a function of the buoyancy effect $g\Delta\rho D$, where g is gravitational acceleration, indicating that a higher pressure difference is need for flooding, or to stop the downward flow, for a larger density effect. Again, this is an expected behavior. However, as mentioned earlier, the pressure differences involved are very small in magnitude and, despite the accuracy of the pressure transducer, a scatter of the data obtained is not surprising. The results were found to be fairly repeatable and the trends observed to be quite consistent. Figure 4 shows the variation of the net volumetric upflow Q_3, which is also equal to the inflow at the side entrance of the tank, with density or pressure difference, keeping the other variable fixed. The observed behavior is physically expected, as discussed earlier.

Several such results have been taken, over wide raqnges of $\Delta\rho$, Δp and L/D. Some correlating equations, giving the flow rates as functions of these variables, have also been derived. Further work is being carried out to improve these to more closely represent the data obtained. In addition, effort is being directed at representing the results in terms of dimensionless variables, such as the Froude number, dimensionless pressure difference, etc. The results support the model developed by Cooper (NISTIR-89-4052, 1989) in terms of the basic trends obtained, the magnitudes of the flow rates and the purging pressure difference, and the relevance of this work to fires in vented enclosures. The next stage in this effort would be to use these results for typical vented rooms, such as those in buildings, ships, etc., and to determine the resulting effect on fire growth and modeling.

Reports and Papers

1. Y. Jaluria and Q. Tan, " Flow Through Horizontal Vents in Compartment Fires," Proc. Fall Tech Meeting, Eastern Sect. Combust. Inst., Orlando, FL, Paper No. 61, 1990.
2. Y. Jaluria, "Flow Through Vents in Room Fires," Ann. Conf. Fire Res., Gaithersburg, MD, October 1990.
3. K. Kapoor and Y. Jaluria, "Mixed Convective Heat Transfer Characteristics of a Downward Turning Buoyant Ceiling Jet, " in Mixed Convection Heat Transfer, ASME Heat Transfer Div., Vol. 163, pp. 9-17, 1991.
4. K. Kapoor and Y. Jaluria, "MIxed Convection Flow Due to a Buoyant Wall Jet Turning Downward at a Corner," in Mixed Convection Heat Transfer, ASME Heat Transfer Div., Vol. 163, pp. 119-128, 1991.
5. K. Kapoor and Y. Jaluria, "Penetrative Natural Convection Flow Due to an Isothermal Vertical surface Immersed in a Thermally Stable Two-layer Environment," ASME Winter Ann. Meet., Atlanta, GA, Dec. 1991, to be presented.
6. Y. Jaluria and K. Kapoor, "Wall and Corner Flows Driven by a Ceiling Jet in an Enclosure Fire," Submitted for publication, 1991.

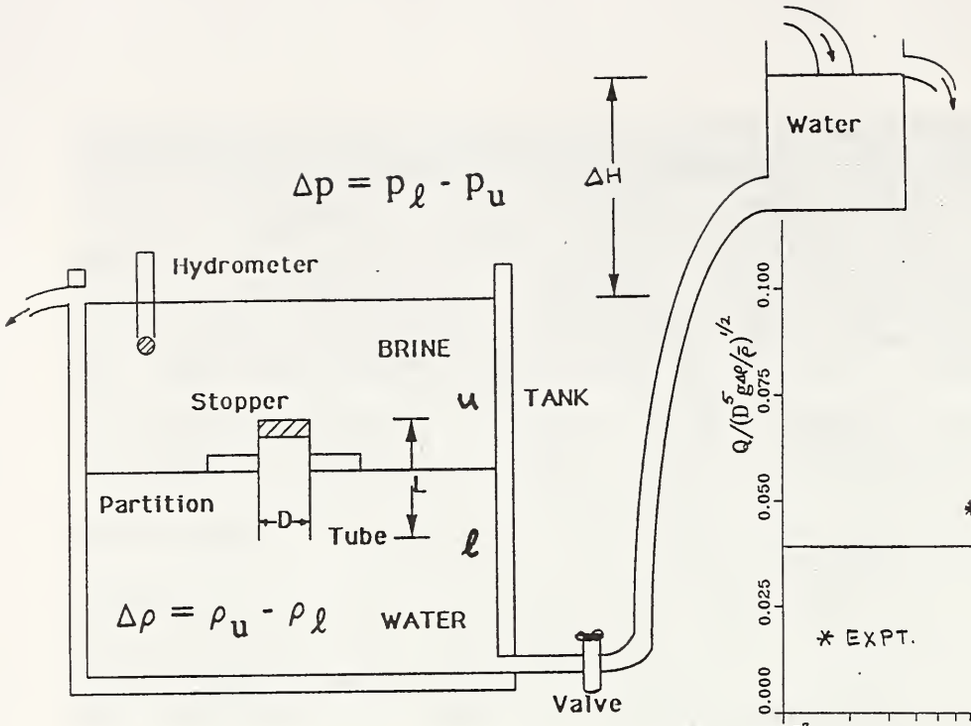


Fig. 1. Sketch of the experimental system.

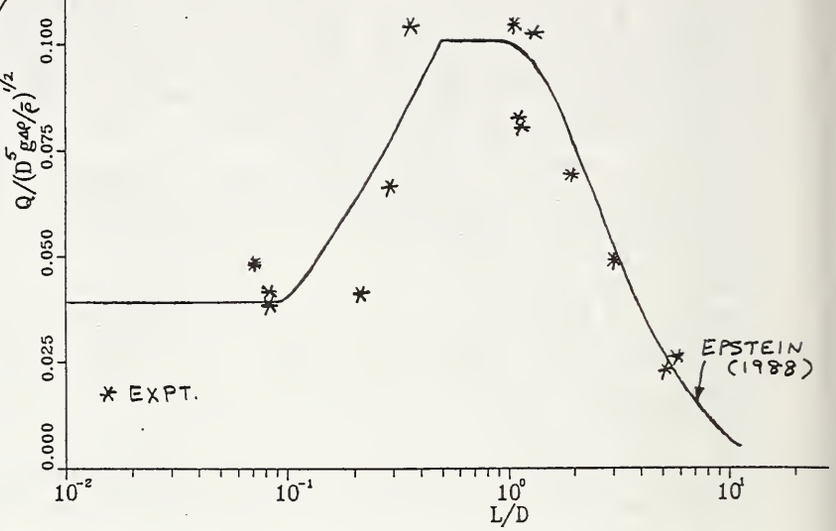
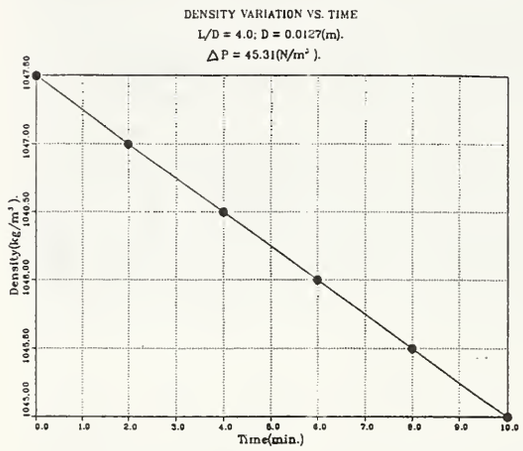


Fig. 2. Comparison between the present data on volume flow rate for $\Delta p = 0$ and those obtained earlier by Epstein (1988).



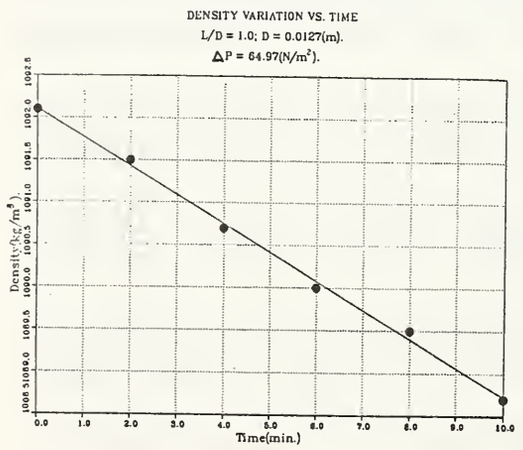
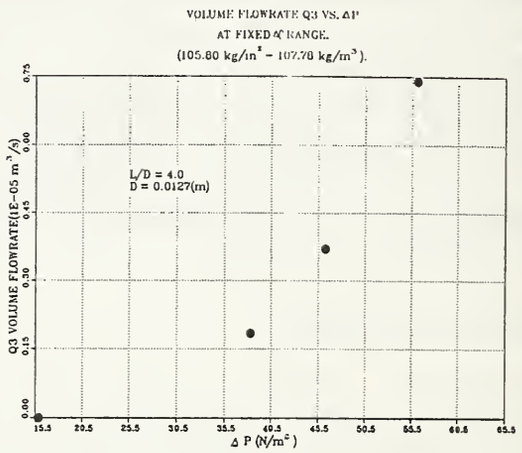


Fig. 3. The variation of the density ρ_u of the upper region fluid with time t for a nonzero pressure difference.



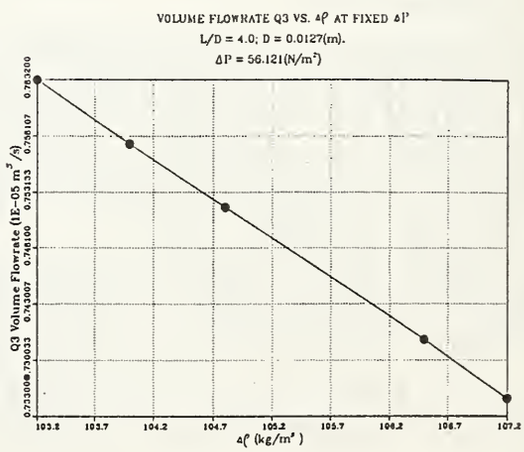


Fig. 4. Measured net upward volume flow rate Q3 for varying pressure and density differences.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

THE DEVELOPMENT OF SPRINKLER EFFECTIVENESS METHODOLOGY FOR THE GSA ENGINEERING FIRE ASSESSMENT SYSTEM

Funding Agency: U.S. General Services Administration

Professional Staff: Daniel Madrzykowski, Project Leader
Robert Vettori, Fire Protection Engineer

Project Objective:
To acquire data on heat release rates required as input to the GSA fire hazard assessment system and develop the methodology to incorporate sprinkler effectiveness into the system.

Technical Accomplishment:
Under the sponsorship of GSA, BFRL has developed an engineering fire hazard assessment system (FPETOOL) to evaluate hazard and fire protection strategies in office/residential occupancies. Although FPETOOL can be used to evaluate a wide range of conditions, it does not specifically address fire suppression. The results of these sprinkler tests are intended to provide a basis for fire suppression prediction in FPETOOL.

Forty-one large scale fire tests were performed under an oxygen consumption calorimetry hood to determine the heat release rate (HRR) of fuel packages with and without sprinklers. Fuel packages included work stations, office furnishings, paper recycling hampers and wooden cribs. Each fuel package was tested under free burn conditions to obtain HRR curves.

The HRR measurements were repeated individually to determine the effect of water spray. The sprinkler was manually activated when the HRR of the fuel package was between 90 and 100 percent of its free burn peak HRR. The average water spray density over the fuel package floor area was 4 mm/min (0.1 gpm/ft^2).

To arrive at the sprinkler effectiveness methodology, the heat release rates measured during suppression were divided by their respective free burn heat release rates. This yielded normalized values for the reduction of HRR for all of the fuel packages. A first order sprinkler effectiveness curve was constructed by determining the maximum normalized HRR, from all of the tested fuel packages, for the 15 minute period after sprinkler activation. Verification testing has been performed to evaluate the limitations of these results as a basis for a sprinkler effectiveness methodology for use in FPETOOL.

Publications :
Development of a Sprinkler Effectiveness Methodology will be published as an NISTIR.

Related Grants:
None

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

EFFECTS OF FIRE SUPPRESSANTS

Funding Agency: Nuclear Regulatory Commission

Professional Staff: Robert S. Levine
Other BFRL staff as required

Project Objective:

Collect data on the effects of fire suppressants on equipment important to safety in nuclear power plants. This is in support of SNL/INEL work on NRC Generic issue 57.

Technical Accomplishments:

Nuclear power plants have many installed fire protection systems. When inadvertant operation occurs, the suppressant (water or CO_2 or Halon are used) may damage operating equipment and/or interfere with safety circuits or create spurious signals. This project used Navy Safety Center data on a large variety of operating system incidents on ships and shore facilities to gain insight into effects that might occur and to enrich the limited statistical data from nuclear power plant experience.

This phase of the project is completed. It was found that the population of inadvertant events in shore facilities parallelled Nuclear Power Plant experience, yielding about 100 cases per year for the 10 years analyzed. This data allowed the Sandia analyst to derive a calculated unreliability about one-fifth that calculated from Nuclear Power Plant experience alone.

It was found that on ships, when sea water was not used, the incidence of damaging effects was much less than the shore facility experience. The fresh water used on ships comes from a closely controlled pure potable water main. So it is postulated that the reason for many of the deleterious effects in Nuclear Power Plants is impure (high electrical conductivity) water. This may be largely due to rust buildup in water residing in sprinkler systems. Incidently, when sea water is used to extinguish fires, there is a very large probability that electrical equipment exposed to it will be damaged.

Follow-on work to test the hypothesis above, and determine how much water impurity can be tolerated in fire protection systems is likely. This will include taking water samples at Nuclear power plants that have had inadvertant discharges with secondary damage and at power plants where secondary damage did not occur. The PI will accompany a Sandia person for some of the early visits. If laboratory work to find out what water purity is needed is found desirable, that work will be done in BFRL, along with confirming a method to measure that purity in the field. The PI will be a project leader for the laboratory work.

Publications:

"Navy Safety Center Data on the Effects of Fire Protection Systems on Electrical Equipment", R.S. Levine, NISTIR 4620, April 1991.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

FIRE AND THERMAL CHARACTERISTICS OF NAVY FIRE FIGHTER TRAINERS

Funding Agency: Naval Training Systems Center, Orlando, Florida

Professional Staff: Robert S. Levine

Project Objective:

Support the development and implementation of prototype fire fighter trainers.

Technical Accomplishments:

Measure air and wall temperatures, atmospheric composition, radiant fluxes, vent flows, and other pertinent characteristics of prototype trainers to evaluate realism and to delineate possible training safety hazards. Prototype trainers are located at Mayport Naval Station, Florida; Groton, Conn., submarine station; Great Lake Naval Station (recruit trainer); Treasure Island (San Francisco); and San Diego. Measurements are made with the BFRL instrument van and/or portable equipment, and the results are reported to the sponsors. Gas species analyses are performed and meetings to discuss them are arranged to obtain site permits from local Environmental Protection Agencies.

On occasion, special analyses are carried out by BFRL and other NIST personnel to obtain information of importance to solve developmental problems. These have included, for instance, metallurgical analysis of slag from a failed smoke generator, electron microscope examination of ceramic insulation to determine the cause of failure, and field equation modeling of possible solutions to problems caused by wind affecting the flames on a carrier deck fire trainer.

Most of the necessary data from the complete stable of prototype trainers have been obtained and analyzed. But the production trainers will use somewhat different burners designed by a different Navy contractor. So measurements will be made to determine whether there are different effects. Also, the concerns of environmental authorities have not all been answered. These will require additional exhaust gas species measurements.

The project leader participates in design reviews, fleet project team meetings, and similar program activities when requested by the sponsor.

Publications:

"Test Plan: Fire and Thermal Characteristics of Mayport 19F Trainers", Levine, R.S., and Rinkinen, W., NISTIR 89-4034, Feb. 1989.

"Exhaust Gas Analysis for Harmful Species: 19F1A Fire Fighting Trainer at Mayport, Florida", Levine, R.S., and Greenaugh, K., NISTIR 4318, May 1990.

BUILDING AND FOR FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

FIRE EVACUATION BY ELEVATORS

Funding Agency

General Services Administration

Professional Personnel

John Klote, Mechanical Engineer, Project Leader
Scot Deal, Fire Protection Engineer
Daniel Alvord, Computer Specialist

Project Objective

Initial study of the feasibility of using elevators for general fire evacuation.

Scope

Fire evacuation by stairs is often very time consuming and not appropriate for many people with physical disabilities. The adaptation of elevators for general fire evacuation is a potential solution to these problems.

Technical Accomplishments

Phase I System Development:

This phase developed conceptual approaches to fire evacuation by elevator including system details, engineering considerations, design analysis, and human behavior considerations. Current techniques of analysis of people movement by elevator have been studied, and methods of analysis of people movement for elevator fire evacuation have been developed. A computer program for analysis of evacuation by elevator has been developed. The human behavior studies of elevator fire evacuation have been started.

Phase II System Evaluation:

The intent of phase II is to analyze elevator evacuation representative buildings by the methods developed in Phase I, and this work will be done next fiscal year.

Reports and Publications

"Design of Elevator Smoke Control Systems for Fire Evacuation," John H. Klote, ASHRAE Transactions, Vol. 97, Part 2.

"Smoke Control for Elevator Evacuation," John H. Klote and George T. Tamura, ASME Symposium on Elevators and Fire Baltimore MD February 19-20, 1991.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

IN-SITU BURNING OF OIL SPILLS

Funding Agency: Minerals Management Service, DoI
U.S. Coast Guard, DoT
American Petroleum Institute

Professional Staff: David D. Evans, Project Leader
William D. Walton, Fire Protection Engineer
Howard R. Baum, NIST Fellow
James H. Morehart, Mechanical Engineer
Kathy A. Notarianni, Fire Protection Engineer
James R. Lawson, General Physical Scientist
Daniel Madrzykowski, Mechanical Engineer
Kurt Keydel, Mechanical Engineer
George W. Mulholland, Research Chemist
Nelson P. Bryner, Chemical Engineer

Project Objective:

To develop and implement the instrumentation and data use methodology for quantifying the combustion of crude oil on water during field experiments of current oil spill burn technology.

Technical Accomplishment:

The development and testing of new measurement equipment and techniques to evaluate crude oil combustion in offshore field tests of in-situ burning involved the use of four different facilities. Two of these facilities are large fire test laboratories and the other two are outdoor liquid fuel burn pans.

Initial laboratory measurements of crude oil burning characteristics were performed in the large fire test facility at NIST. Basic measurements of the combustion process were performed by burning crude oil in 0.4 m and 0.6 m diameter pools and collecting the combustion products in a specially constructed and instrumented exhaust hood system.

The relatively small, 0.6 m diameter, fires studies conducted in BFRL facilities provide a good means of measuring fire characteristics under controlled conditions but are too small to provide an adequate test of measurement equipment under development for field use. Through cooperation with the Fire Research Institute (FRI) in Tokyo, Japan, joint studies of crude oil pool fire burning up to 3 meters in diameter were conducted in the 24 m x 24 m x 20 m high test hall. These tests provided means to evaluate and calibrate sampling equipment developed for field use under controlled laboratory conditions.

As part of the fire fighter training program at the U.S. Navy fire fighter training facility in Norfolk, Virginia, 15 m diameter fuel oil fires are burned and extinguished. These fires were used as burns of opportunity to refine the techniques for instrument transport and positioning in an outdoor wind blown fire plume using tethered mini-blimps controlled by ground crews.

The final stage of preparation for the offshore burns involved the use of fully operational measurement methods in meso-scale crude oil burns up to 15 m square in a specially constructed pan located on Little Sand Island in Mobile Bay. Measurements were completed in Summer, 1991 in a program of 12 meso-scale oil spill burns. In addition to the airborne measurements in the smoke plume, extensive ground measurement equipment was used to characterize the fire thermal radiation field, chemical and particulate species present, and local weather conditions. Data from the studies is still being analyzed. In a preliminary test burn in a 6 m x 6 m corner of the 15 m x 15 m pan, a 45 mm deep layer of Louisiana crude oil on bay water was consumed in 812 seconds. This equates to an average burning velocity of 0.055 mm/s. Smoke yield, the mass fraction of fuel converted to smoke, was found to be 0.14 in this test. This result has increases confidence in the 0.15 smoke yield previously estimated from laboratory measurements as the expected value for smoke yield during from the large crude oil pool fires.

In recent years, advances in computational methods and hardware have made practical the use of techniques to simulate numerically the turbulent mixing of smoke in the atmosphere. In cooperative research between NIST and the Massachusetts Institute of Technology (MIT), a method has been developed to simulate smoke dispersion and settling from crude oil pool fires burning in a uniform wind. This calculation differs from many of the commonly used models of particulate or pollution transport in that no assumptions are made regarding the shape of the smoke density profiles in the plume as it proceeds downwind, nor is any empirical turbulent mixing rule applied. All calculations are based directly on the solutions to the equations of fluid mechanics.

Progress to date allows some useful estimates to be made of particle deposition distances for oil spill burning scenarios. For a crude oil pool of about 2.5×10^3 m^2 area burning in a fire resistant containment boom with an assumed surface regression rate of 5.8×10^{-2} mm/s and a fifteen percent fuel/smoke conversion efficiency, a 18 kg/s mass flux of particulate matter is generated. With an assumed wind speed of 5 m/s and a characteristic length scale for the smoke plume cross section of 300 m, at the height of maximum plume rise, the downwind deposition distance is about 28 km. Doubling the wind speed to 10 m/sec. would bring this distance to 80 km. The width would be approximately 2 km in either case.

Results of this research will be used to prepare for offshore oil spill burning experiments in 1992 and as information for pre-approval of in-situ burning as oil spill response method for various regions of the U.S. and Canada.

Publications :

"Polycyclic Aromatic Hydrocarbon Emissions from the Combustion of Crude Oil on Water," B. A. Benner, Jr., N. P. Bryner, S. A. Wise, G. W. Mulholland, R. C. Lao, M. F. Fingas, Environmental Sciences & Technology, Vol. 24, pp. 1418-1427, (1990).

"Smoke Emission from Burning Crude Oil," D. Evans, W. Walton, H. Baum, G. Mulholland, J. Lawson, H. Koseki, and A. Ghoniem, Proceedings of the Fourteenth Arctic and Marine Oil Spill Program Technical Seminar, June 12-14, 1991, Vancouver, British Columbia, Ministry of Supply and Services Canada, Cat. No. EN 40-11/5-1991, pp. 421-449, (1991).

"Experimental Study of Boilover in Crude Oil Fires," H. Koseki, M. Kokkala, and G. Mulholland, Third International Symposium on Fire Safety Science, Edinburgh, Scotland, (1991).

"Study on Combustion Property of Crude Oil - A Joint Study Between NIST/CFR and FRI," H. Koseki, G. W. Mulholland, and T. Jin, In: Eleventh Joint Panel Meeting of The UJNR Panel on Fire Research and Safety, NISTIR 4449, pp. 96-104, (1990).

"Effect of Diameter on the Burning of Crude Oil Pool Fires," H. Koseki, and G. W. Mulholland, Fire Technology, Vol 27, No. 1, pp. 54-65, (February, 1991)

"Burning of Oil Spills," D. D. Evans, G. W. Mulholland, J. R. Lawson, E. J. Tennyson, P. A. Tebeau, M. F. Fingas, and J. R. Gould, Proceedings of the 1991 Oil Spill Conference (Prevention, Behavior, Control, Cleanup), March 4-7, 1991, San Diego, California, pp 677-680, (1991).

"Field Measurements of Soot Yield Using a Lightweight Sampling System," J. R. Lawson, G. W. Mulholland, and H. Koseki, NISTIR in preparation.

Related Grants:

"Computer Simulation of the Rise, Dispersion and Ground Deposition of Large-Scale Smoke Plumes," Ahmed F. Ghoniem, Massachusetts Institute of Technology.

"A Study of Boilover Mechanism on Crude Oil Combustion," Kozo Saito, University of Kentucky.

BUILDING AND FIRE RESEARCH LABORATORY
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FY91

Institution:	The University of Kentucky
Grant No.:	60NANB1D1123
Grant Title:	A Study of Boilover Mechanism on Crude Oil Combustion
Principal Investigator:	Kozo Saito Associate Professor, Dept. of Mechanical Engineering University of Kentucky Lexington, KY 40506
Other Professional Personnel:	Siru Ling, Master Student Robin Glassburn, UG Student Takao Inamura, Visiting Scientist Akihiko Ito, Visiting Scientist
NIST Scientific Officer:	Dr. Dave Evans

TECHNICAL ABSTRACT:

This study is conducted as part of our continuous effort on study of boilover. Previously, we studied liquid pool fires supported on water sublayer [1-3] and the detailed temperature profiles within fuel and water sublayer using holographic interferometry were reported [3,4]. We conducted this experimental work based on our philosophy: "Observation comes first, then modeling", in other words, "Careful experiments are the source of creativity (modeling)".[5]. The experiments demonstrated that: (1) maximum temperature was achieved 0.1-0.15 mm below the fuel surface due to the in-depth absorption which caused Rayleigh convection in the fuel layer near the surface, and (2) the fuel surface remained at a saturation temperature approximately 20K below the boiling point, while the water at the fuel-water interface was superheated. The superheated water layer is thermodynamically unstable, so that sporadic spatterings of water and fuel droplets (boilover) were observed. Interferograms taken at the onset of boiling in the water sublayer [3] shows the detailed temperature structure in the fuel and water sublayer.

To prevent accidental occurrence of the boilover and develop a technique to prevent it, the detailed mechanisms of the boilover should be understood. To that end, we visualized the boilover process in a well controlled laboratory-scale experiment; and the results were recorded using a 35mm still camera and a video camera/record system. We observed nucleation

through active/sporadic boiling of the water sublayer by changing the silicon oil layer thickness from 1.5 to 6 mm under a fixed fire level heat flux (1.5 W/cm^2).

Silicon was chosen because it has high boiling point(approximately 500K) and non-combustible ensuring safety during the experiment. We found that the most intense boiling occurred for the silicon oil thickness, 1.5 and 3 mm, while with increasing the silicon oil thickness the degree of the boiling decreased. For the 6mm silicon oil thickness, the bubble formation became less frequent and the distance of spatterings of oil and water droplets which was caused by the superheated water vapor became shorter. We also observed that there is two kinds of boiling, "weak" boiling and "strong" boiling. The weak boiling is a moderate process composed of frequent repetition of nucleation and eruption of small bubbles. The strong boiling is associated with a sudden eruption of the superheated water vapor accumulated under the silicon oil layer and is less frequent. But when it occurs, it involves the eruption of the whole interface and splashing of a large amount of oil and water to the surrounding of the container. The nature of the strong boiling is similar to the boilover observed for the large scale pool fires [1].

In order to develop a technique to prevent the boilover, it is important to find a method to suppress the occurrence of the strong boiling. One way to do this is to add a small amount of fine particles at the silicon-water interface to enhance the process of small bubble nucleation which can help to release the superheated vapor energy moderately. We sprinkled small amount of fine polymer particles (its density is 0.98 g/cm^3 and they are thermally and chemically stable up to 400K) on the water surface and permormed a boilover experiment. As we expected, addition of the particles enhanced the small bubble nucleation resulting in faster nucleation compared to the case without particles. However, the particles did not prevent the occurrence of the strong boiling, thus further research is needed.

EXPERIMENTAL METHOD

Boilover is a very complicated phenomenon when it occurs in a large scale fire of crude oils supported on water, since the flame is turbulent and the combustion process is highly transient because the crude oils contain low flash point components to high boiling point residues. To simplify these complications with keeping the essential boilover mechanism as equal as possible to the large scale, we designed a small scale pool fire test apparatus. The container was made from an aluminum cylinder (inner diameter is 15 cm and height is 17.5 cm) with a concentric water cooling cylinder and a PMMA bottom to observe the boiling phenomenon. The temperature of the container wall was kept approximately at the room temperature by circulating water in the annual cylinder space to prevent nucleation of boiling at the wall. A cone heater which can provide a constant and uniform

heat flux at the silicon oil surface up to 8 W/cm^2 was used to simulate the flame. The cone heater was constructed based on the prototype design provided by the National Institute of Standards and Technology. Its usefulness for fire research has been well documented by Babrauskas [6]. On top of the water sublayer we placed a layer of silicon oil which is noncombustible and whose boiling point is above 500K (thus, it is ideal for our experimental purpose). After the cone heater achieved a steady state heat flux, it was applied to the silicon surface. Temperature of the silicon and water layers were measured using Chromel-Alumel thermocouples placed at several different depths along the center line from the silicon open surface. Boilover phenomenon was observed through the bottom surface with a mirror which was located underneath the container and reflected the image in 90 degree angle.

First four different silicon oil thickness (0.15, 0.3, 0.45 and 0.6 cm) were tested using a constant heat flux at the silicon oil surface (1.5 W/cm^2) without particles on the water surface. Then the same series of experiments were repeated by equally sprinkling small amount of fine polymer particles on the water surface. Onset time of nucleation and of active boiling were measured from the recorded video film. Here, the onset of nucleation is defined as the time when one bubble appeared at the silicon-water interface, and the onset of boiling is defined as the time when whole silicon-water interface is involved in boiling.

SOME RESULTS

We summarized experimental results in Table 1 which indictes the effect of small particles for the onset of nucleation and active boiling. For the silicon oil thickness of 1.5 mm, the effect of particles are not significant, thus the time of nucleation and active boiling are almost the same, but the particles significantly delayed the time of occurrence of a strong boiling. For the silicon oil thickness of 3.0, these times became shorter for the case with particles due to the enhanced nucleation by the particles. The particles also made a delay of occurrence of the strong boiling approximately five minutes. For the silicon oil thickness of 4.5 mm, the onset of water bubble nucleation with particles occurred in 8 minutes shorter than that without particles and again the particles delayed the occurrence of a strong boiling. For the silicon oil thickness of 6.0 mm, there is no difference concerning the onset time of boiling. However, the onset of nucleation with particles occurred 7 minutes earlier than that without particles and again particles delayed the occurrence of a strong boiling significantly. As a result, we found that addition of the small particles at the water surface shorten the onset of nucleation, and delayed the occurrence of a strong boiling significantly.

Table 1 Experimental results

Silicon Oil Thickness (mm):	1.5	3.0	4.5	6.0
Without particles				
Onset of nucleation (min.):	5.5	11	22	28
Onset of boiling (min.):	8.5	19	34	40
With particles				
Onset of nucleation (min.):	5.0	8.0	14	21
Onset of boiling (min.):	9.0	18	28	40

REFERENCES

[1] Arai,M., Saito,K. and Altenkirch,R.A., C.S.T., 71:25 (1990).
[2] Inamura,T., Saito,K. and Tagavi,K.A., C.S.T., (submitted).
[3] Ito,A., Masuda,D. and Saito,K., Comb. Flame, 83:375 (1991).
[4] Ito,A., Inamura,T., Saito,K. and Evans,D., 3rd ASME/JSME Thermal Engg. Conf., Reno, NE, 1991, and submitted to J. Heat Transfer.
[5] Saito, K., "The Role of Observation in Scientific Research" and "Application of Zen's Philosophy to Increase Creativity", to be published.
[6] Babrauskas,V., J.Fire Mater., 8:81 (1984).

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT-1991

MEASUREMENT OF CONDITIONS RESULTING FROM A FLAMING FIRE IN A SIMULATED NIH HOSPITAL ROOM PROTECTED BY AUTOMATIC FIRE SPRINKLERS

Funding Agency: National Institutes of Health

Professional Staff: Kathy A. Notarianni, Project Leader
W. Douglas Walton, Fire Protection Engineer
Robert Vettori, Fire Protection Engineer

Project Objective:

To generate a data bank of measured fire exposures and combustion product concentrations occurring at the patient location, as well as activation times of various automatic sprinklers and smoke detectors for NIH so that it can be determined if smoke detectors should be used to alert nursing staff prior to the activation of the sprinklers.

Technical Accomplishments:

The minimum size flaming fire in terms of rate of heat release that could cause potentially harmful conditions in a patient room was determined through propane burner tests in a simulated NIH Clinical Center Hospital room along with computer modeling using Hazard I, and FPE tool. 60 kw was determined to be the critical fire size.

Burns of various fuel packages were conducted under a calorimeter in order to identify a package with a nominal 60 kw rate of heat release. This was determined to be a wood crib approximately 18" X 24" X 6" high, weighing about 17 lbs.

A series of 5 full-scale tests were conducted to measure temperatures, radiation, and carbon dioxide, carbon monoxide, and oxygen concentrations resulting from the flaming wood crib fires within the simulated NIH Clinical Center Hospital room protected with automatic sprinklers. Extensive records of test measurements were taken which include measured time for activation of smoke detectors and "dry" sprinkler heads located throughout the room.

A Report of Test, "Five Small Flaming Fire Tests in a Simulated Hospital Patient Room Protected by Automatic Fire Sprinklers", Notarianni, Kathy A., October 1990 was issued.

Related Grants:
None

BUILDING AND FOR FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
OTHER AGENCY PROJECT - 1991

STAGING AREAS FOR PEOPLE WITH PHYSICAL DISABILITIES

Funding Agency

General Services Administration

Professional Personnel

John Klote, Mechanical Engineer, Project Leader
Scot Deal, Fire Protection Engineer
Daniel Alvord, Computer Specialist

Project Objective

Develop the capability to evaluate the fire safety of staging areas for people with physical disabilities.

Scope

The fire safety of the handicapped in multi-story buildings is a matter of considerable concern, and staging areas are one approach that has gained considerable attention for providing fire safety. This project develops a method for evaluating the safety of the staging area concept.

Technical Accomplishments

A method of evaluation of the threat within staging areas was developed including methods analysis of smoke transport and tenability analysis for staging areas. This method included the development of a general method and computer routine for analysis of stack effect. Field tests were conducted of the six GSA buildings in which staging areas have been installed to study the smoke protection performance of the systems. Human behavior studies consisted of observing fire drills in the six buildings to gain information about the extent to which these systems will be accepted and used as intended. The importance of occupant and visitor training is obvious from these studies. The information gained by these studies will be applied to the six GSA buildings.

Reports and Publications

"A General Routine for Analysis of Stack Effect," John H. Klote, National Institute of Standards and Technology, NISTIR 4588.

Related Grant

"Effectiveness of Staging Areas in Office Buildings", Carl M. Harris, George Mason University.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
FY91

Institution: George Mason University

Grant No.: 50SBNB1C6527

Grant Title: Effectiveness of Staging Areas in Office Buildings

Principal Investigator: Prof. Carl M. Harris, Chairman
Dept. of Operations Research & Applied Statistics
George Mason University
4400 University Drive
Fairfax, VA 22030-4444

Other Professional Personnel: Dr. Bernard M. Levin
Dr. Norman E. Groner

NIST Scientific Officer: Dr. John Klote

Technical Abstract:

Objectives. One approach for assuring the safety of disabled occupants of office buildings, in a fire emergency, is to provide a staging area or an area of refuge where the disabled occupants can wait safely until either they can be assisted out of the building or the fire is extinguished. The General Services Administration (GSA) of the Federal Government is retrofitting six office buildings with staging areas to upgrade the fire safety for disabled occupants: three in Washington, DC; one in Toledo, OH; one in St. Paul, MN; and one in Bemidji, MN. This provides a unique opportunity to evaluate the value of staging areas as an approach for providing a high level of actual safety; to evaluate the perceived safety of the office buildings by the disabled occupants; and to develop guidelines for implementing future systems. The thrust of this project is the human factors aspects of fire protection systems that use staging areas.

Preliminary Criteria. Dr. Groner developed a set of Preliminary Criteria for Evaluating the Use of Refuge Areas. These criteria are being used in evaluating the occupant related aspects of the staging areas in the six buildings. Conversely, the information obtained is being used to evaluate and modify the Preliminary Criteria. These Criteria contain factors that should be considered in establishing Staging Areas. They address three major areas of concern: development of a fire safety plan which clearly targets those individuals who should use the staging areas and ensures their safety; refinement and implementation of the plan through consultations with fire department personnel and building occupants and through appropriate training exercises; and distribution to occupants of a written plan in which the most vital information is clearly conveyed. We expect to change these Criteria editorially and submit them to the General Services Administration for use in guiding the future establishment of staging areas in GSA office buildings.

Copies of the Preliminary Criteria were sent to appropriate officials in the six buildings prior to site visits. This was done to provide the officials with some ideas that they might wish to implement prior to our arrival. It would also alert the officials as to what we would be looking for during the site visits.

Site Visits. Drs. Norman Groner and Bernard Levin visited the six GSA Buildings recently retrofitted with staging areas. These site visits included:

Tours of the buildings to observe and become familiar with the staging areas.

Discussions with the responsible officials.

Interviews with building occupants, especially those with disabilities and those who fill emergency roles (e.g. floor wardens.)

Observations of fire drills.

Status of the Installations. The installations are all quite new. In fact, it was not clear to what extent the physical installations were complete and accepted by GSA. They all appeared to be sufficiently completed that they could be used. In most buildings the fire plan was in the process of being updated and modified. In several of the buildings the fire safety plan had not yet been updated to include the new staging areas. A final report will be prepared after we receive copies of the updated fire safety plans and we have an opportunity to revisit the Washington Buildings, preferably in conjunction with the scheduled October 1991 fire drills.

Characteristics of the Won-Doors. Five of the six buildings had special sliding or curtain doors to separate most of the small staging areas from the corridors. This special type of fire door is called a Won-Door, a horizontal sliding door, or a Fireguard Door. It is designed to protect the staging areas from fires in the corridors (1.5 hour fire rating). Won-Doors are usually used to protect openings considerably larger than the entrances to the small staging areas. The project addressed the changes that are required for use in protecting relatively small openings. The original design of the door appears to have allowed its use for both large and small settings. However, the installed doors included options specifically designed for large openings. The relative merits of a properly designed Won-Door as compared with traditional fire doors are being addressed.

BUILDING AND FIRE RESEARCH LABORATORY
FIRE RESEARCH PROGRAM
FY91

TECHNICAL SUPPORT FOR 'SUPER 301' TRADE AGREEMENT

Professional Personnel

Vytenis Babrauskas, Project leader
Kenneth Steckler

Project Objective

To provide technical consultation and advice on fire and earthquake testing to U.S. delegation to the Super 301 U.S.-Japan trade agreement.

Sponsor

National Forest Products Association

Technical Approach

This project is geared towards the successful implementation by Japan of new building code provisions and fire test standards which permit 3-storey construction using wood 2x4 techniques.

NIST role will be to proved technical advice and guidance as needed, so that full-scale earthquake + fire tests carried out by BRI to a consensually agreed-upon plan can meet with successful results. As a side benefit, possible guidance may be derived from this program for needed changes to U.S. code provisions or test standards.

The major experimental activity is a full-scale earthquake and fire test of a 3-storey house, to be conducted at the Building Research Institute, Tsukuba, Japan. NIST cooperative activities will center around:

1. Measurement of leakage through earthquake-racked walls.

2. Mapping of wall cracks in order to establish a relationship between earthquake damage and fire failures.

3. Cone Calorimeter testing of products used in construction, in order to establish use of heat release rate measurements for replacing traditional tests for non-combustibility.

4. Exploration of logical problems in code approach to fire endurance versus non-combustibility.

5. Review of US and Canadian code bases for set-back provisions, in order to reflect on any additional data input which might be useful for the Japanese code.

6. Examine the Japanese modifications to the ISO fire endurance standard, ISO 834, with an eye to determining if they may have applicability outside of Japan.

7. Computer modeling of predicted fire.

3.0 Alphabetical Listing of BFRL Fire Research Grantees and Their Grants

3.0 **Alphabetical Listing of BFRL Fire Research Grantees and Their Grants**

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